Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:13 pm BST

PDB ID	:	2QF7
Title	:	Crystal structure of a complete multifunctional pyruvate carboxylase from Rhizobium etli
Authors	:	St Maurice, M.; Surinya, K.H.; Rayment, I.
Deposited on	:	2007-06-27
Resolution	:	2.00 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:

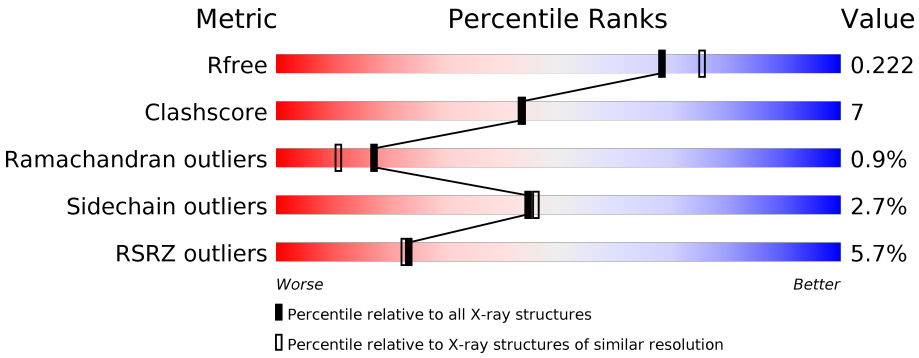
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	1165	5% 79% 12% •• 8%
1	B	1165	5% 78% 8% • 13%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17618 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 Pyruvate carboxylase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1076	Total	C	N	O	S	0	31	0
			8286	5271	1411	1573	31			
1	B	1017	Total	C	N	O	S	0	33	0
			7896	5030	1342	1493	31			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q2K340
A	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-3	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
A	0	GLY	-	EXPRESSION TAG	UNP Q2K340
A	1	GLY	-	EXPRESSION TAG	UNP Q2K340
A	718	KCX	LYS	MODIFIED RESIDUE	UNP Q2K340
B	-10	MET	-	EXPRESSION TAG	UNP Q2K340
B	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-3	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
B	0	GLY	-	EXPRESSION TAG	UNP Q2K340
B	1	GLY	-	EXPRESSION TAG	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	718	KCX	LYS	MODIFIED RESIDUE	UNP Q2K340

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

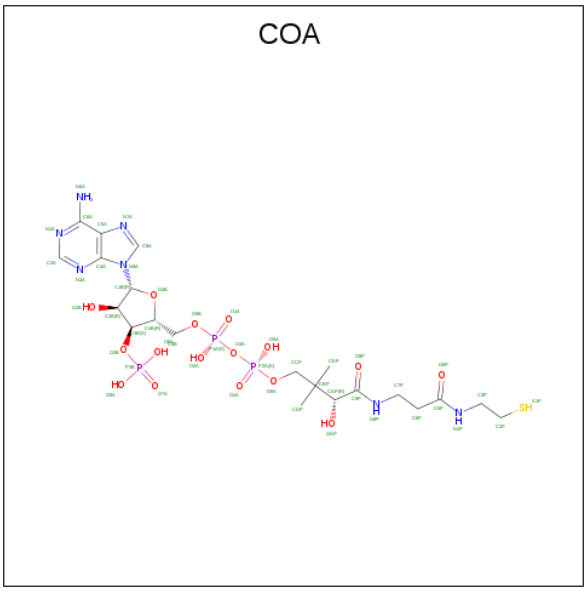
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

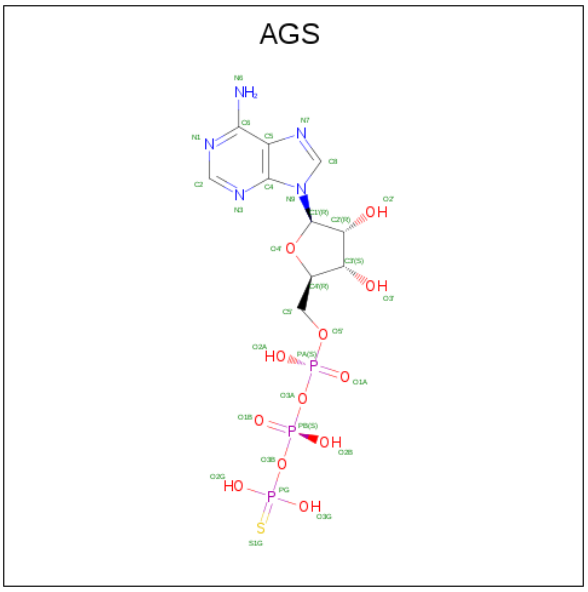
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	A	2	Total Cl 2 2	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



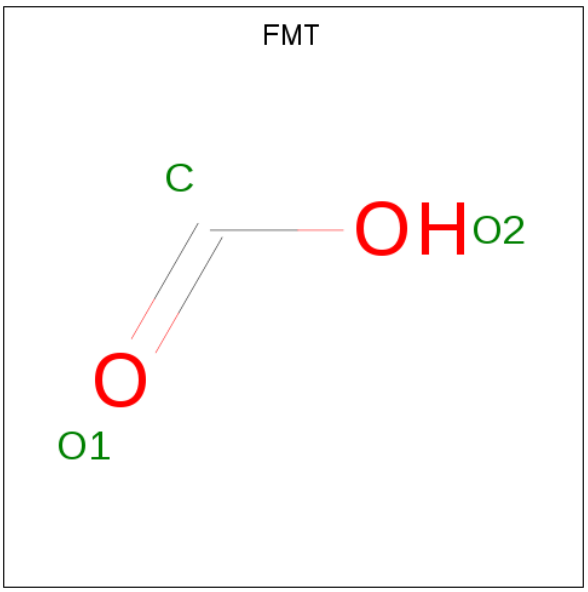
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



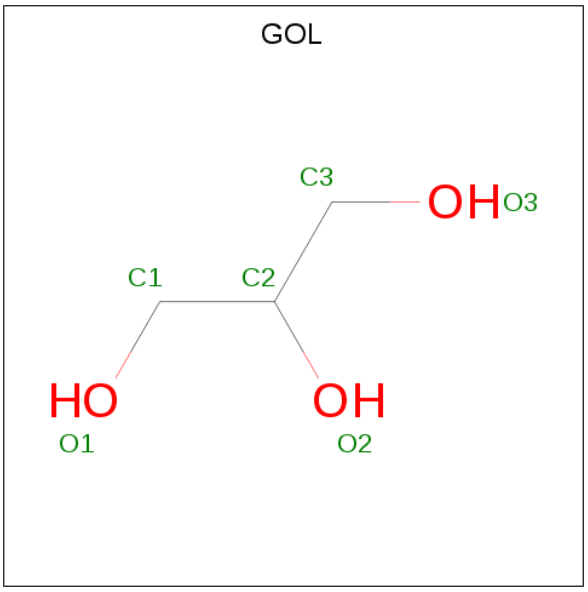
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
6	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

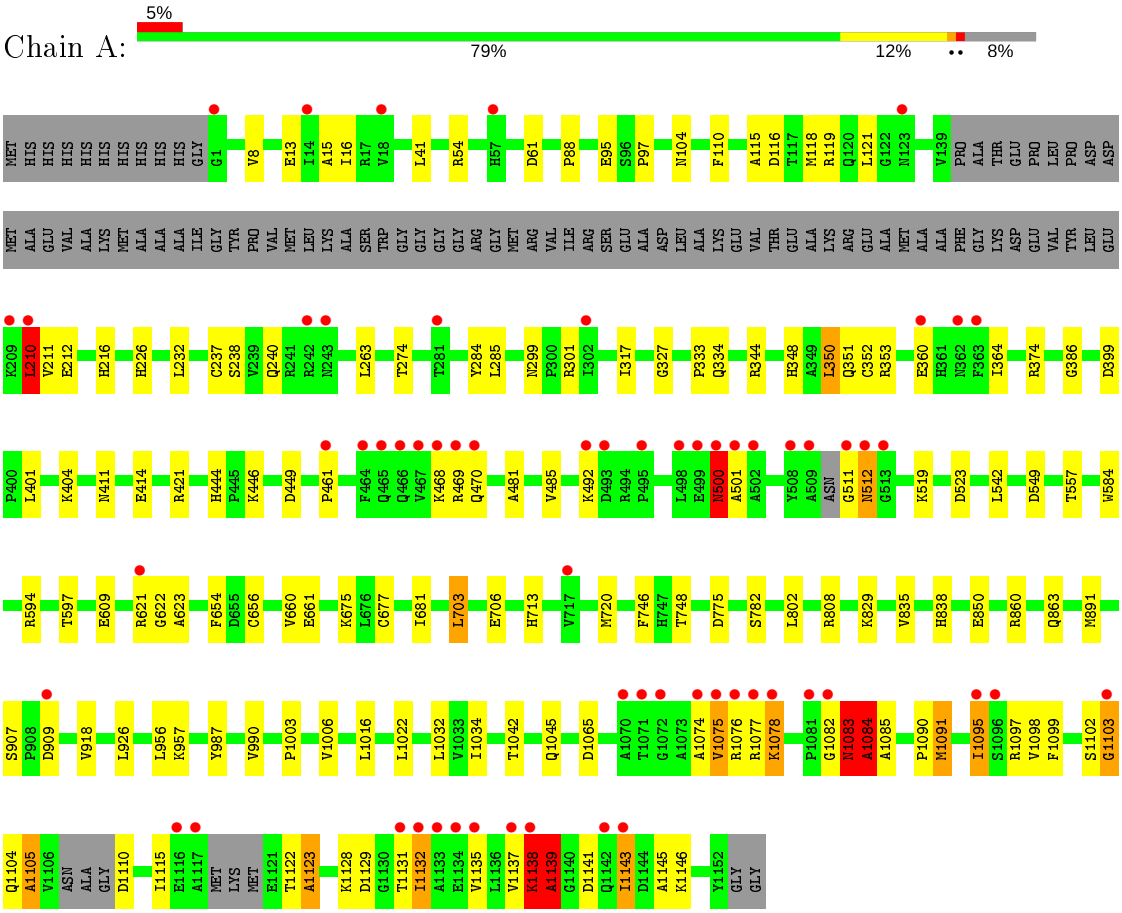
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	687	Total O 687 687	0	0
9	B	631	Total O 631 631	0	0

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.

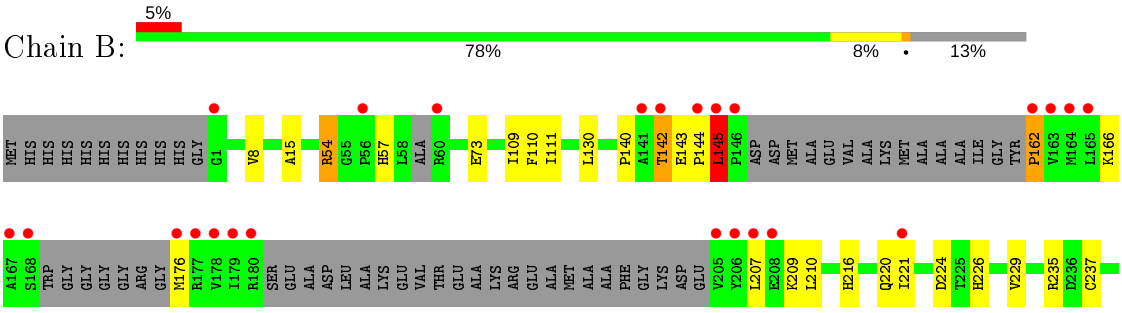
- Molecule 1: Pyruvate carboxylase protein

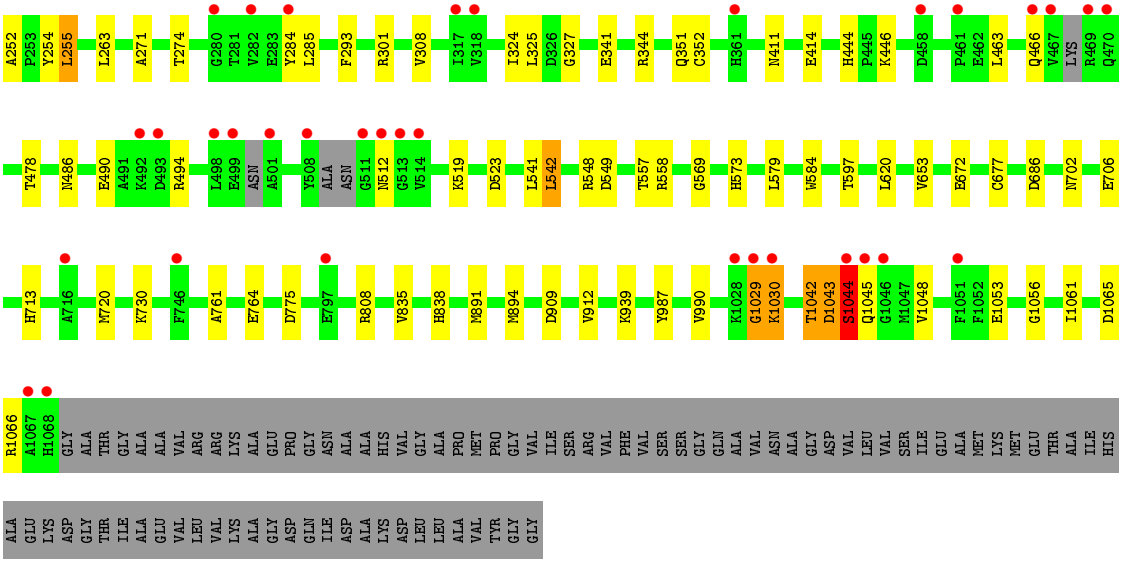
Chain A:



- Molecule 1: Pyruvate carboxylase protein

Chain B:




A252 P253 Y254 L255 L263 A271 T274 G280 T281 V282 E283 Y284 L285 F293 R301 V308 I317 V318 I324 L325 D326 G327 E341 R344 Q351 C352 H361 N411 E414 H444 P445 K446 D458 P461 E462 L463 Q466 V467 LYS R469 Q470
T478 N486 E490 A491 K492 D493 R494 L498 E499 ASN A501 Y508 ALA ASN G511 N512 G513 V514 K519 D523 L541 L542 R548 D549 T557 R558 G569 H573 L579 W584 T597 L620 V653 E672 C677 D686 N702 E706
H713 A716 M720 K730 F746 A761 E764 D775 E797 R808 V835 H838 M891 M894 D909 V912 K939 Y987 V990 K1028 G1029 K1030 T1042 D1043 S1044 Q1045 G1046 H1047 V1048 F1051 F1052 E1053 G1056 I1061 D1065
R1066 A1067 H1068 GLY ALA THR GLY ALA ALA ALA VAL ARG ARG LYS ALA ALA GLU PRO GLY ASN ALA ALA HIS VAL GLY ALA PRO MET PRO GLY VAL ILE SER ARG VAL PHE VAL SER SER GLY GLN ALA VAL ASN ALA GLY ASP VAL LEU VAL SER ILE GLU ALA MET LYS MET GLU GLY THR ALA ILE HIS
ALA GLU LYS ASP GLY THR ILE ALA GLU VAL LEU VAL LYS ALA ALA GLY ASP GLN ILE ASP ALA ALA LYS ASP LEU LEU ALA VAL TYR GLY GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	234.73Å 93.26Å 137.22Å 90.00° 107.33° 90.00°	Depositor
Resolution (Å)	131.31 – 2.00 29.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (131.31-2.00) 96.9 (29.70-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.223 0.178 , 0.222	Depositor DCC
R_{free} test set	9277 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17618	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CL, FMT, ZN, COA, AGS, KCX

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	0.78	1/8518 (0.0%)	0.79	9/11577 (0.1%)
1	B	0.76	0/8107	0.76	12/11005 (0.1%)
All	All	0.77	1/16625 (0.0%)	0.77	21/22582 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	675	LYS	CE-NZ	5.53	1.62	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	145	LEU	CA-CB-CG	7.64	132.87	115.30
1	A	1139	ALA	N-CA-C	6.95	129.78	111.00
1	A	549	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	350	LEU	CA-CB-CG	6.60	130.47	115.30
1	B	301	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	285	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	B	549	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	542	LEU	CA-CB-CG	-5.67	102.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352[A]	CYS	CA-CB-SG	5.57	124.02	114.00
1	B	352[B]	CYS	CA-CB-SG	5.57	124.02	114.00
1	A	594	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	B	686	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	1084	ALA	N-CA-C	5.23	125.12	111.00
1	A	350	LEU	CB-CG-CD1	5.21	119.85	111.00
1	B	549	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	548	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	301	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	1103	GLY	N-CA-C	5.02	125.65	113.10
1	B	1044	SER	N-CA-C	-5.01	97.46	111.00
1	A	374	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	686	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1074	ALA	Peptide
1	A	1083	ASN	Peptide
1	A	1084	ALA	Peptide
1	A	1138	LYS	Peptide
1	A	1139	ALA	Peptide
1	B	1029	GLY	Peptide
1	B	1043	ASP	Peptide
1	B	1044	SER	Peptide
1	B	162	PRO	Peptide

5.2 Too-close contacts (i)

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	8286	0	8122	136	0
1	B	7896	0	7704	78	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	32	0	11	4	0
6	A	31	0	12	0	0
6	B	31	0	12	0	0
7	A	3	0	1	0	0
7	B	3	0	1	0	0
8	B	6	0	8	0	0
9	A	687	0	0	15	0
9	B	631	0	0	10	0
All	All	17618	0	15871	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (214) 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:1139:ALA:HB1	1:A:1141:ASP:H	0.99	1.14
1:A:1137:VAL:HA	1:A:1138:LYS:CB	1.79	1.11
1:A:1095:ILE:HG12	1:A:1139:ALA:HB3	1.28	1.09
1:A:511:GLY:HA2	1:A:512:ASN:HB2	1.33	1.09
1:A:210:LEU:HB3	1:A:211:VAL:CA	1.87	1.03
1:B:909:ASP:OD2	9:B:1468:HOH:O	1.76	1.00
1:A:95:GLU:C	1:A:118[A]:MET:HE1	1.83	0.99
1:A:210:LEU:CB	1:A:211:VAL:HA	1.90	0.99
1:A:1084:ALA:N	1:A:1085:ALA:HB3	1.79	0.97
1:A:511:GLY:HA2	1:A:512:ASN:CB	1.95	0.97
1:A:210:LEU:HB3	1:A:211:VAL:HA	0.99	0.96
1:B:677:CYS:H	1:B:713:HIS:HD2	1.04	0.96
1:A:1077:ARG:HA	1:A:1078:LYS:HB2	1.45	0.95
1:A:808:ARG:HD3	9:A:1304:HOH:O	1.67	0.95
1:A:1137:VAL:CA	1:A:1138:LYS:CB	2.47	0.92
1:A:1139:ALA:HB1	1:A:1141:ASP:N	1.85	0.90
1:A:500:ASN:H	1:A:500:ASN:ND2	1.63	0.90
1:A:500:ASN:N	1:A:500:ASN:HD22	1.63	0.89
1:A:104:ASN:ND2	9:A:1578:HOH:O	1.96	0.88
1:A:500:ASN:HB2	1:A:501:ALA:CA	2.04	0.88
1:A:511:GLY:CA	1:A:512:ASN:HB2	2.05	0.85
1:B:341[A]:GLU:OE1	9:B:1411:HOH:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HG13	1:B:351[A]:GLN:HE21	1.42	0.84
1:A:1084:ALA:H	1:A:1085:ALA:HB3	1.43	0.84
1:B:808[B]:ARG:HD3	9:B:1334:HOH:O	1.76	0.84
1:A:1095:ILE:HD11	1:A:1098:VAL:HG23	1.62	0.79
1:A:95:GLU:O	1:A:118[A]:MET:HE1	1.81	0.79
1:B:220:GLN:HE21	1:B:235:ARG:HH12	1.31	0.78
1:A:1122:THR:HA	1:A:1123:ALA:HB3	1.67	0.77
1:B:677:CYS:H	1:B:713:HIS:CD2	1.97	0.77
1:A:1095:ILE:HG12	1:A:1139:ALA:CB	2.13	0.77
1:A:1139:ALA:CB	1:A:1141:ASP:H	1.92	0.75
1:A:677:CYS:H	1:A:713:HIS:HD2	1.34	0.75
1:A:621[C]:ARG:NE	9:A:1331:HOH:O	2.18	0.75
1:A:500:ASN:H	1:A:500:ASN:HD22	0.82	0.75
1:A:621[C]:ARG:NH1	9:A:1749:HOH:O	2.20	0.75
1:A:216:HIS:CD2	1:A:237:CYS:HB2	2.21	0.75
1:A:1095:ILE:CG1	1:A:1139:ALA:HB3	2.14	0.73
1:A:1138:LYS:CB	1:A:1141:ASP:OD2	2.39	0.71
1:B:490:GLU:OE1	1:B:558[B]:ARG:NH1	2.17	0.71
1:B:142:THR:CG2	1:B:207:LEU:H	2.03	0.70
1:A:444:HIS:HD2	1:A:446:LYS:H	1.40	0.70
1:A:1095:ILE:HD11	1:A:1098:VAL:CG2	2.20	0.70
1:B:111:ILE:HA	1:B:325[A]:LEU:HD22	1.73	0.70
1:B:730[A]:LYS:HE3	1:B:761:ALA:HA	1.72	0.70
1:A:860:ARG:HH11	1:A:863:GLN:HE22	1.40	0.69
1:B:130:LEU:HD21	1:B:274:THR:HG22	1.75	0.69
1:A:1045:GLN:HE21	1:A:1076:ARG:H	1.41	0.68
1:B:486:ASN:ND2	1:B:1066:ARG:H	1.92	0.68
1:B:216:HIS:CD2	1:B:237:CYS:HB2	2.29	0.67
1:B:1042:THR:HG21	1:B:1065:ASP:OD2	1.95	0.67
1:A:210:LEU:HG	1:A:212:GLU:H	1.58	0.67
1:B:486:ASN:HD21	1:B:1066:ARG:H	1.43	0.67
1:A:542[B]:LEU:HD22	1:A:802:LEU:CD1	2.25	0.67
1:B:519:LYS:NZ	1:B:523:ASP:OD2	2.27	0.67
1:B:808[A]:ARG:NH1	9:B:1788:HOH:O	2.28	0.67
1:A:1045:GLN:NE2	1:A:1076:ARG:H	1.92	0.66
1:A:621[C]:ARG:HD3	1:A:622:GLY:N	2.11	0.66
1:A:1122:THR:HA	1:A:1123:ALA:CB	2.26	0.66
1:B:226:HIS:HE1	1:B:327:GLY:O	1.78	0.66
1:A:1097:ARG:HD2	1:A:1099:PHE:CE2	2.32	0.65
1:A:1083:ASN:HD22	1:A:1083:ASN:H	1.45	0.64
1:B:130:LEU:HD21	1:B:274:THR:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HG13	1:B:351[A]:GLN:NE2	2.13	0.64
1:A:621[C]:ARG:HG2	1:A:621[C]:ARG:HH21	1.63	0.63
1:A:891[B]:MET:CE	1:A:918:VAL:HG11	2.28	0.63
1:A:1077:ARG:CA	1:A:1078:LYS:HB2	2.24	0.63
1:B:1029:GLY:H	1:B:1030:LYS:HB2	1.63	0.63
1:A:1097:ARG:HD2	1:A:1099:PHE:CZ	2.34	0.63
1:A:121:LEU:HD21	1:A:274:THR:HG21	1.78	0.63
1:A:1135:VAL:HG12	1:A:1137:VAL:O	1.98	0.62
1:A:444:HIS:CD2	1:A:446:LYS:H	2.17	0.62
1:A:621[A]:ARG:HG2	1:A:654:PHE:CZ	2.35	0.62
1:B:142:THR:HG22	1:B:207:LEU:H	1.64	0.62
1:A:364:ILE:HD13	1:A:1082:GLY:HA2	1.81	0.61
1:B:444:HIS:HD2	1:B:446:LYS:H	1.49	0.61
1:A:1105:ALA:HB3	1:A:1110:ASP:OD1	2.00	0.61
1:B:411[B]:ASN:ND2	1:B:414:GLU:H	1.99	0.60
1:B:490:GLU:O	1:B:494:ARG:HD2	2.01	0.60
1:A:621[C]:ARG:HH21	1:A:621[C]:ARG:CG	2.15	0.60
1:A:1095:ILE:HG22	1:A:1143:ILE:HD13	1.84	0.60
1:A:97:PRO:HD3	1:A:118[A]:MET:HE2	1.84	0.60
1:B:229:VAL:HG11	1:B:271:ALA:CB	2.32	0.59
1:A:1115:ILE:N	1:A:1122:THR:O	2.27	0.58
1:A:677:CYS:H	1:A:713:HIS:CD2	2.18	0.58
1:A:681:ILE:HG23	1:A:703[A]:LEU:HD23	1.86	0.57
1:A:850:GLU:OE2	9:A:1536:HOH:O	2.18	0.57
1:B:263[B]:LEU:HD11	1:B:284:TYR:CD2	2.39	0.57
1:A:232:LEU:CD2	1:A:317[A]:ILE:HD11	2.34	0.57
1:A:511:GLY:CA	1:A:512:ASN:CB	2.74	0.57
1:A:808:ARG:NE	9:A:1527:HOH:O	1.99	0.56
1:A:481:ALA:O	1:A:485:VAL:HG13	2.06	0.56
1:B:569:GLY:O	1:B:573:HIS:HD2	1.89	0.56
1:B:142:THR:HG21	1:B:207:LEU:H	1.71	0.56
1:B:894:MET:HE3	1:B:912:VAL:HG13	1.86	0.56
1:A:609[B]:GLU:HG2	9:A:1346:HOH:O	2.06	0.56
1:A:621[C]:ARG:NH2	1:A:656:CYS:H	2.04	0.55
1:B:229:VAL:HG11	1:B:271:ALA:HB3	1.87	0.55
1:A:8:VAL:HG11	1:A:15:ALA:HA	1.89	0.55
1:A:95:GLU:O	1:A:118[A]:MET:CE	2.55	0.54
1:A:1084:ALA:H	1:A:1085:ALA:CB	2.19	0.54
1:A:511:GLY:HA2	1:A:512:ASN:CG	2.27	0.54
1:A:449:ASP:OD2	9:A:1469:HOH:O	2.18	0.54
1:B:987:TYR:HB3	1:B:990:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621[C]:ARG:CD	9:A:1331:HOH:O	2.55	0.54
1:B:1044:SER:O	1:B:1045:GLN:HB2	2.09	0.53
1:B:8:VAL:HG11	1:B:15:ALA:HA	1.91	0.53
1:B:166:LYS:HG2	1:B:176:MET:HG3	1.91	0.52
1:A:542[B]:LEU:HD22	1:A:802:LEU:HD12	1.91	0.52
1:B:1029:GLY:N	1:B:1030:LYS:HB2	2.24	0.52
1:B:1029:GLY:HA3	1:B:1030:LYS:CG	2.40	0.52
1:B:444:HIS:CD2	1:B:446:LYS:H	2.28	0.52
1:A:621[C]:ARG:HD3	9:A:1331:HOH:O	2.09	0.52
1:A:333:PRO:HG2	1:A:334:GLN:NE2	2.25	0.51
1:A:1045:GLN:CB	1:A:1075:VAL:HG22	2.41	0.51
1:A:353:ARG:HG2	1:A:404:LYS:HG2	1.91	0.51
1:B:254:TYR:CE1	1:B:255:LEU:HD13	2.46	0.51
1:A:1145:ALA:O	1:A:1146:LYS:HB2	2.11	0.51
1:A:621[C]:ARG:CD	1:A:623:ALA:H	2.24	0.51
1:B:702:ASN:O	1:B:706[A]:GLU:HG3	2.11	0.51
1:B:57:HIS:CE1	1:B:73:GLU:OE1	2.64	0.50
1:A:1045:GLN:HB3	1:A:1075:VAL:HG22	1.93	0.50
1:B:143:GLU:O	1:B:145:LEU:N	2.44	0.50
1:B:109:ILE:CG2	1:B:325[A]:LEU:HD23	2.42	0.50
1:A:226:HIS:HE1	1:A:327:GLY:O	1.95	0.49
1:A:1032:LEU:HD21	5:A:1161:COA:H1B	1.94	0.49
1:A:987:TYR:HB3	1:A:990:VAL:HB	1.94	0.49
1:A:621[B]:ARG:HG2	1:A:654:PHE:CE2	2.48	0.49
1:A:411[A]:ASN:ND2	1:A:414:GLU:H	2.11	0.49
1:A:333:PRO:HG2	1:A:334:GLN:HE22	1.78	0.49
1:A:713:HIS:HE1	9:A:1508:HOH:O	1.96	0.49
1:A:1083:ASN:HD22	1:A:1083:ASN:N	2.11	0.48
1:A:16:ILE:HG23	9:B:1586:HOH:O	2.14	0.48
1:A:1103:GLY:CA	1:A:1131:THR:HA	2.44	0.48
1:A:1003:PRO:O	1:A:1006:VAL:HG22	2.14	0.48
1:A:621[A]:ARG:HG2	1:A:654:PHE:CE2	2.48	0.47
1:B:110:PHE:O	1:B:325[A]:LEU:HD21	2.13	0.47
1:B:730[A]:LYS:HE2	1:B:764:GLU:HB3	1.95	0.47
1:B:57:HIS:HE1	1:B:73:GLU:OE1	1.97	0.47
1:A:1137:VAL:CB	1:A:1138:LYS:CB	2.92	0.47
1:B:209:LYS:HG2	1:B:210:LEU:N	2.29	0.47
1:B:730[A]:LYS:HG2	1:B:761:ALA:HB1	1.97	0.47
1:A:808:ARG:NH2	9:A:1527:HOH:O	2.48	0.46
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.50	0.46
1:A:835:VAL:HA	1:A:838:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ILE:CD1	1:A:1135:VAL:HG22	2.46	0.46
1:A:41:LEU:HD12	1:A:386:GLY:O	2.15	0.46
1:A:746:PHE:CZ	1:A:748:THR:HB	2.51	0.46
1:A:95:GLU:CA	1:A:118[A]:MET:HE1	2.45	0.46
1:A:677:CYS:N	1:A:713:HIS:HD2	2.09	0.46
1:A:470:GLN:HB2	5:A:1161:COA:O2A	2.16	0.45
1:A:1122:THR:CA	1:A:1123:ALA:HB3	2.42	0.45
1:A:461:PRO:HD2	9:A:1786:HOH:O	2.15	0.45
1:B:730[A]:LYS:HE3	1:B:761:ALA:CA	2.44	0.45
1:B:730[A]:LYS:HD2	9:B:1441:HOH:O	2.16	0.45
1:A:118[A]:MET:HB3	1:A:118[A]:MET:HE2	1.59	0.45
1:B:1042:THR:HB	1:B:1048:VAL:CG2	2.46	0.45
1:A:660:VAL:HG11	1:A:706[A]:GLU:HG2	1.99	0.45
1:B:308:VAL:H	1:B:351[A]:GLN:NE2	2.15	0.44
1:A:232:LEU:HD22	1:A:317[A]:ILE:HD11	1.98	0.44
1:B:110:PHE:O	1:B:325[A]:LEU:CD2	2.65	0.44
1:A:351:GLN:HG2	1:A:352:CYS:N	2.32	0.44
1:B:224:ASP:HA	1:B:324:ILE:HG23	2.00	0.44
1:B:1053:GLU:OE1	1:B:1056:GLY:HA2	2.18	0.44
1:A:263:LEU:HD11	1:A:284:TYR:CD2	2.53	0.43
1:A:621[B]:ARG:HG2	1:A:654:PHE:CZ	2.54	0.43
1:B:54:ARG:HD3	9:B:1495:HOH:O	2.18	0.43
1:B:221:ILE:HD13	1:B:271:ALA:HB2	1.99	0.43
1:A:1090:PRO:HG2	1:A:1091:MET:CE	2.49	0.43
1:B:162:PRO:O	1:B:210:LEU:N	2.49	0.43
1:A:621[C]:ARG:CZ	1:A:656:CYS:H	2.31	0.43
1:B:220:GLN:NE2	1:B:235:ARG:HH12	2.07	0.43
1:A:238:SER:O	1:A:240:GLN:HG3	2.18	0.43
1:A:519[A]:LYS:NZ	1:A:523:ASP:OD2	2.52	0.43
1:B:252:ALA:HB3	1:B:255:LEU:HD22	2.00	0.43
1:A:1022[A]:LEU:HD11	1:A:1034:ILE:HD12	2.00	0.42
1:A:1105:ALA:O	1:A:1129:ASP:CA	2.66	0.42
1:A:1042:THR:OG1	1:A:1065:ASP:OD2	2.35	0.42
1:B:142:THR:HG23	1:B:143:GLU:O	2.19	0.42
1:B:226:HIS:CE1	1:B:327:GLY:O	2.66	0.42
1:A:1084:ALA:O	1:A:1128:LYS:HD3	2.18	0.42
1:A:1137:VAL:HB	1:A:1138:LYS:CB	2.49	0.42
1:B:730[B]:LYS:HD3	9:B:1426:HOH:O	2.19	0.42
1:A:1016:LEU:HD21	1:A:1022[A]:LEU:HD23	2.01	0.42
1:A:421:ARG:HD2	1:A:421:ARG:C	2.40	0.42
1:A:54:ARG:HD3	1:A:61:ASP:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621[B]:ARG:HB3	1:A:621[B]:ARG:CZ	2.50	0.42
1:B:730[A]:LYS:CE	1:B:764:GLU:HB3	2.49	0.42
1:A:1084:ALA:N	1:A:1085:ALA:CB	2.66	0.41
1:A:1122:THR:CA	1:A:1123:ALA:CB	2.96	0.41
1:B:1029:GLY:HA3	1:B:1030:LYS:CB	2.50	0.41
1:B:891:MET:HE3	1:B:894:MET:HE2	2.00	0.41
1:A:348:HIS:HD2	9:A:1189:HOH:O	2.02	0.41
1:B:478:THR:HA	1:B:1061:ILE:HG21	2.02	0.41
1:B:894:MET:HE3	1:B:912:VAL:CG1	2.50	0.41
1:B:254:TYR:CD1	1:B:255:LEU:HD13	2.55	0.41
1:A:115:ALA:O	1:A:119:ARG:HG3	2.20	0.41
1:A:469:ARG:HB3	5:A:1161:COA:O5A	2.21	0.41
1:B:541:LEU:HB3	1:B:579:LEU:HB2	2.03	0.41
1:A:1103:GLY:HA2	1:A:1131:THR:HA	2.03	0.41
1:A:621[C]:ARG:HH22	1:A:656:CYS:HB3	1.85	0.41
1:B:263[A]:LEU:HD21	1:B:293:PHE:CD1	2.56	0.41
1:B:1029:GLY:CA	1:B:1030:LYS:HB2	2.51	0.40
1:B:411[B]:ASN:HD21	1:B:414:GLU:H	1.66	0.40
1:A:88:PRO:HG3	1:A:110:PHE:CZ	2.56	0.40
1:B:620:LEU:O	1:B:653:VAL:HA	2.20	0.40
1:A:1032:LEU:HD23	5:A:1161:COA:N3A	2.36	0.40
1:A:621[C]:ARG:HH22	1:A:656:CYS:H	1.67	0.40
1:A:782:SER:HA	9:A:1477:HOH:O	2.21	0.40
1:B:672:GLU:CG	9:B:1419:HOH:O	2.70	0.40
1:A:1095:ILE:CG2	1:A:1139:ALA:HB3	2.51	0.40
1:A:1095:ILE:HG23	1:A:1139:ALA:CB	2.51	0.40
1:B:713:HIS:HE1	9:B:1535:HOH:O	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1096/1165 (94%)	1055 (96%)	29 (3%)	12 (1%)	14 8
1	B	1032/1165 (89%)	1001 (97%)	24 (2%)	7 (1%)	22 16
All	All	2128/2330 (91%)	2056 (97%)	53 (2%)	19 (1%)	17 11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	512	ASN
1	A	1138	LYS
1	B	145	LEU
1	B	1044	SER
1	A	500	ASN
1	A	1078	LYS
1	A	1105	ALA
1	A	1123	ALA
1	B	144	PRO
1	B	1030	LYS
1	A	468	LYS
1	A	492	LYS
1	A	957	LYS
1	A	1104	GLN
1	B	1043	ASP
1	A	1075	VAL
1	B	512	ASN
1	B	140	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	843/934 (90%)	813 (96%)	30 (4%)	35 34
1	B	803/934 (86%)	787 (98%)	16 (2%)	55 58
All	All	1646/1868 (88%)	1600 (97%)	46 (3%)	44 44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	116	ASP
1	A	210	LEU
1	A	285	LEU
1	A	299	ASN
1	A	344	ARG
1	A	350	LEU
1	A	360	GLU
1	A	401	LEU
1	A	500	ASN
1	A	557	THR
1	A	584	TRP
1	A	597	THR
1	A	661[A]	GLU
1	A	661[B]	GLU
1	A	703[A]	LEU
1	A	703[B]	LEU
1	A	720	MET
1	A	775	ASP
1	A	829	LYS
1	A	907	SER
1	A	909	ASP
1	A	926	LEU
1	A	956	LEU
1	A	1083	ASN
1	A	1091	MET
1	A	1095	ILE
1	A	1102	SER
1	A	1132	ILE
1	A	1143	ILE
1	B	54	ARG
1	B	142	THR
1	B	145	LEU
1	B	255	LEU
1	B	344	ARG
1	B	463[A]	LEU
1	B	463[B]	LEU
1	B	466	GLN
1	B	542	LEU
1	B	557	THR
1	B	584	TRP
1	B	597	THR

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Mol	Chain	Res	Type
1	B	720	MET
1	B	775	ASP
1	B	939	LYS
1	B	1042	THR

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	129	ASN
1	A	226	HIS
1	A	240	GLN
1	A	334	GLN
1	A	348	HIS
1	A	351	GLN
1	A	444	HIS
1	A	486	ASN
1	A	500	ASN
1	A	630	ASN
1	A	713	HIS
1	A	863	GLN
1	A	898	GLN
1	A	1045	GLN
1	A	1083	ASN
1	B	57	HIS
1	B	220	GLN
1	B	226	HIS
1	B	228	ASN
1	B	339	ASN
1	B	348	HIS
1	B	361	HIS
1	B	444	HIS
1	B	486	ASN
1	B	536	ASN
1	B	573	HIS
1	B	713	HIS
1	B	847	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	KCX	A	718[A]	1,3	7,11,12	1.16	1 (14%)	4,12,14	0.58	0
1	KCX	B	718[A]	1,3	7,11,12	1.05	0	4,12,14	2.11	1 (25%)

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	A	718[A]	1,3	-	1/7/10/12	-
1	KCX	B	718[A]	1,3	-	1/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718[A]	KCX	CE-NZ	2.57	1.51	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	718[A]	KCX	CE-NZ-CX	3.69	129.20	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\|>2$
7	FMT	B	1163	-	0,2,2	0.00	-	0,1,1	0.00	-
6	AGS	A	1162	2	26,33,33	2.40	6 (23%)	26,52,52	1.42	6 (23%)
8	GOL	B	1162	-	5,5,5	0.28	0	5,5,5	0.63	0
5	COA	A	1161	-	29,34,50	1.17	2 (6%)	34,53,75	1.33	2 (5%)
6	AGS	B	1161	2	26,33,33	2.38	6 (23%)	26,52,52	1.48	4 (15%)
7	FMT	A	1163	-	0,2,2	0.00	-	0,1,1	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
6	AGS	A	1162	2	-	8/17/38/38	0/3/3/3
6	AGS	B	1161	2	-	4/17/38/38	0/3/3/3
8	GOL	B	1162	-	-	2/4/4/4	-
5	COA	A	1161	-	-	6/20/40/64	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1162	AGS	PG-O2G	7.43	1.79	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1162	AGS	PG-O3G	7.33	1.78	1.54
6	B	1161	AGS	PG-O2G	7.31	1.78	1.54
6	B	1161	AGS	PG-O3G	6.93	1.77	1.54
5	A	1161	COA	C2A-N3A	4.02	1.38	1.32
6	B	1161	AGS	C5-C4	3.19	1.49	1.40
6	A	1162	AGS	C5-C4	3.15	1.49	1.40
6	B	1161	AGS	C2-N3	2.82	1.36	1.32
6	B	1161	AGS	O4'-C1'	2.60	1.44	1.41
6	B	1161	AGS	PG-S1G	2.56	1.96	1.90
5	A	1161	COA	C2A-N1A	2.41	1.38	1.33
6	A	1162	AGS	PG-S1G	2.38	1.95	1.90
6	A	1162	AGS	C2-N3	2.36	1.35	1.32
6	A	1162	AGS	O4'-C1'	2.22	1.44	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1161	COA	N3A-C2A-N1A	-5.94	119.39	128.68
6	B	1161	AGS	N3-C2-N1	-3.69	122.91	128.68
6	A	1162	AGS	N3-C2-N1	-3.38	123.40	128.68
6	B	1161	AGS	O2G-PG-O3B	2.97	114.54	104.64
5	A	1161	COA	C5B-C4B-C3B	-2.69	105.47	114.40
6	B	1161	AGS	N6-C6-N1	2.66	124.09	118.57
6	B	1161	AGS	C2-N1-C6	2.62	123.24	118.75
6	A	1162	AGS	O2G-PG-O3B	2.55	113.14	104.64
6	A	1162	AGS	C4-C5-N7	-2.48	106.81	109.40
6	A	1162	AGS	C2-N1-C6	2.19	122.50	118.75
6	A	1162	AGS	C3'-C2'-C1'	2.18	104.26	100.98
6	A	1162	AGS	PA-O3A-PB	-2.12	125.55	132.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1162	AGS	PB-O3B-PG-O2G
6	A	1162	AGS	C5'-O5'-PA-O1A
6	A	1162	AGS	C5'-O5'-PA-O2A
6	A	1162	AGS	O4'-C4'-C5'-O5'
6	A	1162	AGS	C3'-C4'-C5'-O5'
6	B	1161	AGS	PB-O3B-PG-O2G
5	A	1161	COA	CCP-O6A-P2A-O4A
8	B	1162	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	1162	AGS	PB-O3A-PA-O2A
6	B	1161	AGS	PB-O3A-PA-O2A
5	A	1161	COA	CCP-O6A-P2A-O3A
8	B	1162	GOL	O2-C2-C3-O3
5	A	1161	COA	CCP-O6A-P2A-O5A
6	A	1162	AGS	PB-O3B-PG-O3G
6	B	1161	AGS	PB-O3A-PA-O1A
6	B	1161	AGS	O4'-C4'-C5'-O5'
6	A	1162	AGS	C5'-O5'-PA-O3A
5	A	1161	COA	P1A-O3A-P2A-O4A
5	A	1161	COA	P1A-O3A-P2A-O5A
5	A	1161	COA	C5B-O5B-P1A-O1A

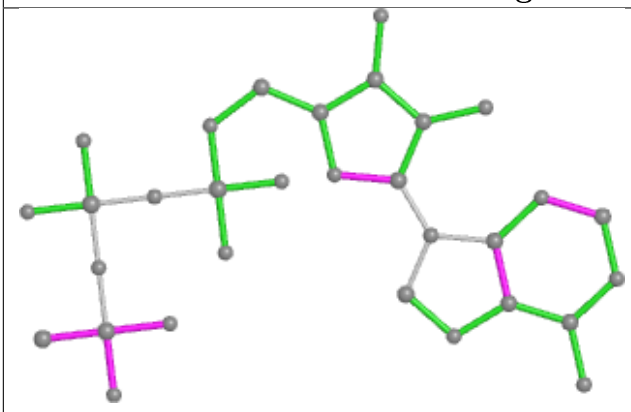
There are no ring outliers.

1 monomer is involved in 4 short contacts:

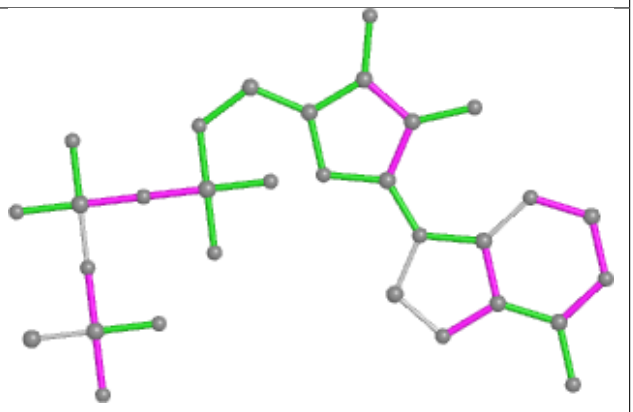
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1161	COA	4	0

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 then 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.

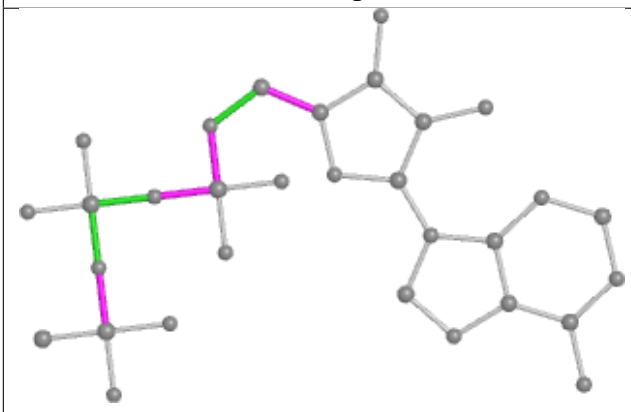
Ligand AGS A 1162



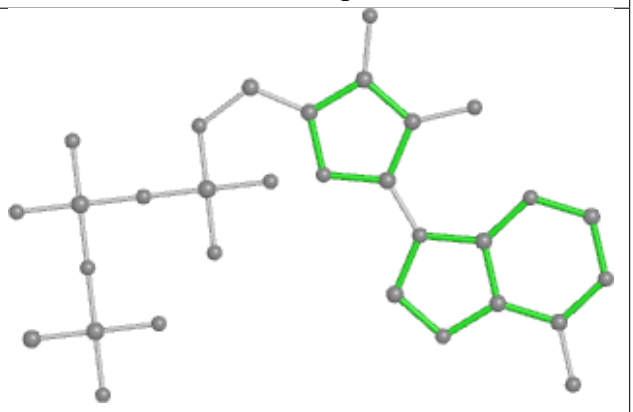
Bond lengths



Bond angles

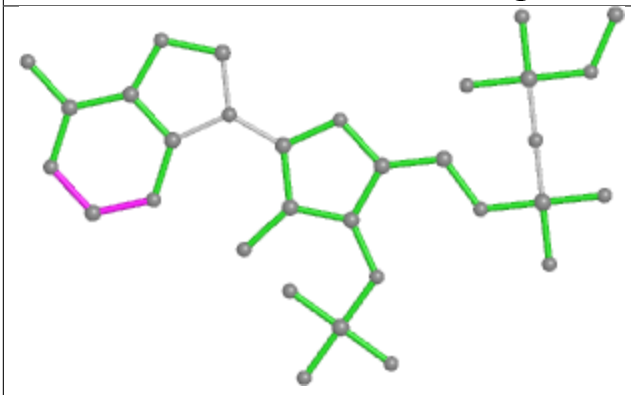


Torsions

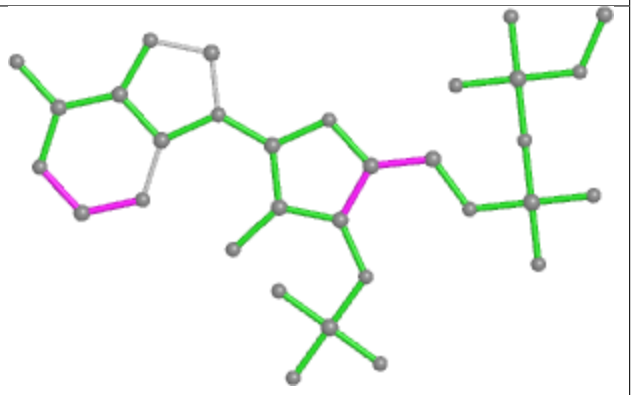


Rings

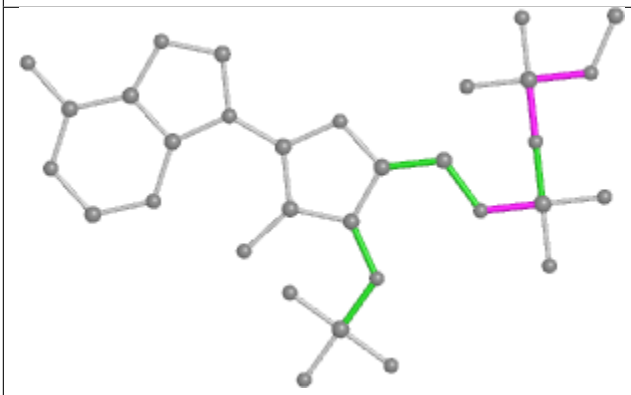
Ligand COA A 1161



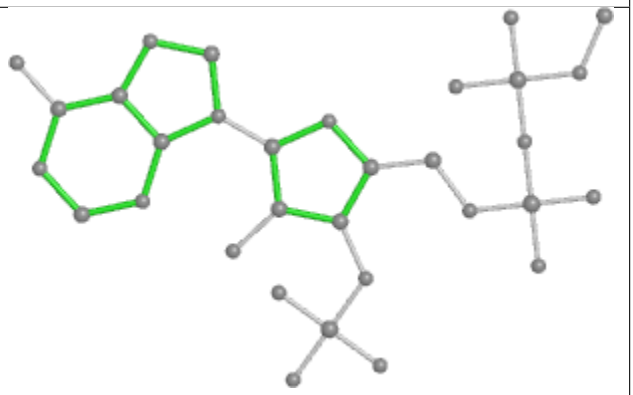
Bond lengths



Bond angles

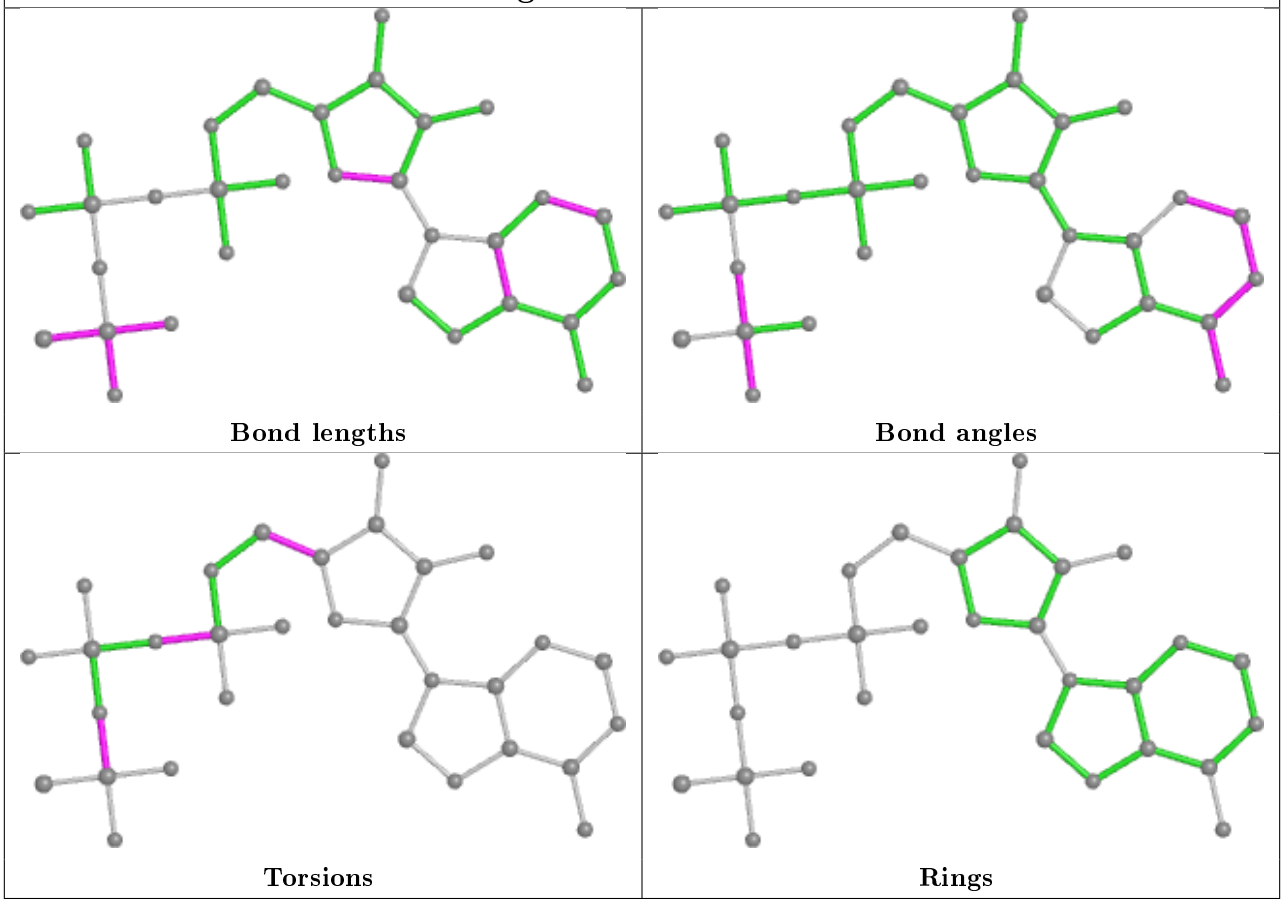


Torsions



Rings

Ligand AGS B 1161



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^{th} 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	1075/1165 (92%)	0.10	62 (5%)	23	22	11, 24, 37, 52	13 (1%)
1	B	1016/1165 (87%)	0.12	58 (5%)	23	23	16, 24, 40, 64	8 (0%)
All	All	2091/2330 (89%)	0.11	120 (5%)	23	23	11, 24, 38, 64	21 (1%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	PRO	10.3
1	B	145	LEU	7.7
1	B	207	LEU	7.5
1	A	467	VAL	7.3
1	B	179	ILE	6.7
1	A	509	ALA	6.3
1	B	513	GLY	5.7
1	B	1044	SER	5.6
1	B	56	PRO	5.5
1	B	1068	HIS	5.5
1	A	512	ASN	5.4
1	B	167	ALA	5.3
1	B	144	PRO	5.3
1	B	178	VAL	5.1
1	B	1029	GLY	5.1
1	A	1075	VAL	5.0
1	A	1	GLY	4.8
1	B	141	ALA	4.8
1	B	467	VAL	4.7
1	B	508	TYR	4.7
1	A	210	LEU	4.6
1	B	142	THR	4.6
1	A	500	ASN	4.5
1	A	511	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	162	PRO	4.4
1	A	1071	THR	4.4
1	A	501	ALA	4.4
1	B	511	GLY	4.3
1	B	1045	GLN	4.3
1	B	499	GLU	4.3
1	B	165	LEU	4.3
1	A	1074	ALA	4.2
1	A	508	TYR	4.2
1	A	1082	GLY	4.1
1	B	206	TYR	4.1
1	A	468	LYS	3.9
1	A	1081	PRO	3.9
1	B	205	VAL	3.9
1	B	176	MET	3.8
1	A	1133	ALA	3.8
1	B	512	ASN	3.7
1	A	498	LEU	3.6
1	A	1131	THR	3.6
1	A	1072	GLY	3.6
1	A	502	ALA	3.4
1	A	466	GLN	3.3
1	B	466	GLN	3.3
1	B	177	ARG	3.3
1	B	469	ARG	3.3
1	A	1137	VAL	3.2
1	B	493	ASP	3.2
1	B	1028	LYS	3.2
1	B	501	ALA	3.2
1	A	470	GLN	3.2
1	A	513	GLY	3.1
1	B	163	VAL	3.1
1	B	164	MET	3.1
1	B	282	VAL	3.1
1	A	492	LYS	3.0
1	A	909	ASP	3.0
1	B	498	LEU	3.0
1	A	363	PHE	3.0
1	A	469	ARG	3.0
1	A	1103	GLY	2.9
1	B	1067	ALA	2.9
1	A	1143	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1078	LYS	2.8
1	B	458	ASP	2.8
1	A	1132	ILE	2.8
1	A	1077	ARG	2.7
1	A	1134	GLU	2.7
1	A	360	GLU	2.7
1	A	302	ILE	2.6
1	A	242	ARG	2.6
1	A	1076	ARG	2.6
1	B	797[A]	GLU	2.5
1	B	168	SER	2.5
1	B	317	ILE	2.5
1	A	1070	ALA	2.5
1	B	461	PRO	2.5
1	A	499	GLU	2.5
1	A	209	LYS	2.5
1	B	470	GLN	2.5
1	B	716	ALA	2.4
1	B	280	GLY	2.4
1	A	243	ASN	2.4
1	B	1051[A]	PHE	2.4
1	A	1117	ALA	2.3
1	A	465	GLN	2.3
1	A	362	ASN	2.3
1	A	461	PRO	2.3
1	B	60	ARG	2.3
1	A	464	PHE	2.3
1	B	208	GLU	2.3
1	A	717	VAL	2.3
1	B	1	GLY	2.3
1	A	1116	GLU	2.2
1	A	1138	LYS	2.2
1	A	18	VAL	2.2
1	A	495	PRO	2.2
1	A	493	ASP	2.2
1	B	492	LYS	2.2
1	B	1046	GLY	2.2
1	B	180	ARG	2.2
1	A	1095	ILE	2.2
1	B	1030	LYS	2.2
1	A	1142	GLN	2.1
1	A	57	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	ILE	2.1
1	B	221	ILE	2.1
1	B	514	VAL	2.1
1	A	621[A]	ARG	2.1
1	B	318	VAL	2.1
1	A	281	THR	2.1
1	B	361	HIS	2.1
1	B	284	TYR	2.1
1	A	123	ASN	2.0
1	A	1096	SER	2.0
1	A	1135	VAL	2.0
1	B	746	PHE	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, 95^{th} 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
1	KCX	A	718[A]	12/13	0.91	0.20	21,23,25,27	0
1	KCX	B	718[A]	12/13	0.94	0.20	21,23,28,29	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. The B-factors column lists the minimum, median, 95^{th} 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
6	AGS	A	1162	31/31	0.77	0.25	36,48,50,52	12
6	AGS	B	1161	31/31	0.79	0.21	24,39,43,44	9
2	MG	A	1156	1/1	0.83	0.21	39,39,39,39	0
8	GOL	B	1162	6/6	0.83	0.21	30,34,39,46	0

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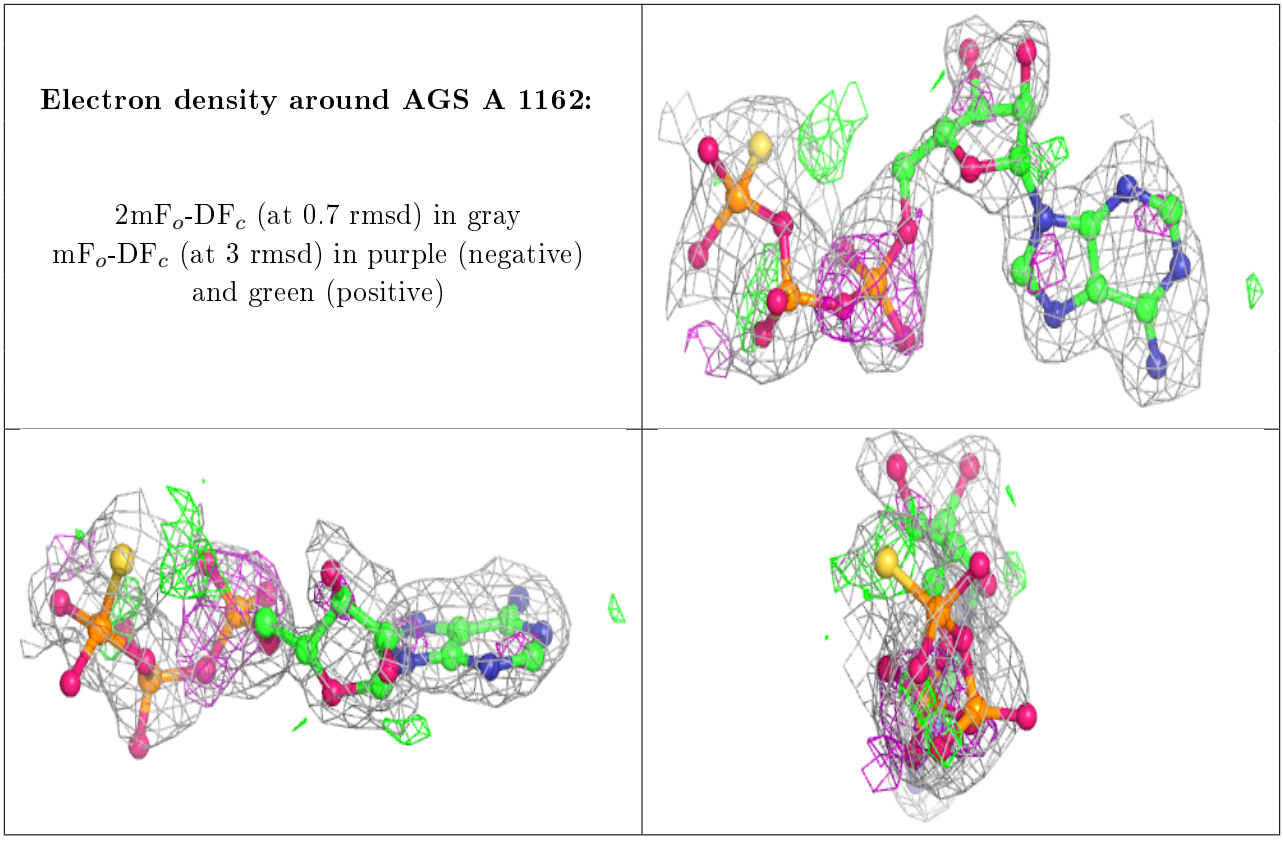
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	COA	A	1161	32/48	0.88	0.19	16,20,25,27	32
2	MG	B	1158	1/1	0.93	0.14	24,24,24,24	0
2	MG	A	1155	1/1	0.94	0.06	13,13,13,13	1
4	CL	B	1160	1/1	0.94	0.15	38,38,38,38	0
2	MG	B	1157	1/1	0.95	0.16	34,34,34,34	0
4	CL	B	1159	1/1	0.97	0.17	28,28,28,28	0
2	MG	B	1156	1/1	0.98	0.04	20,20,20,20	0
2	MG	A	1158	1/1	0.98	0.20	17,17,17,17	0
4	CL	A	1160	1/1	0.98	0.23	35,35,35,35	0
7	FMT	A	1163	3/3	0.98	0.10	18,18,19,19	0
7	FMT	B	1163	3/3	0.99	0.11	18,18,18,19	0
3	ZN	A	1157	1/1	0.99	0.06	15,15,15,15	0
4	CL	A	1159	1/1	0.99	0.20	24,24,24,24	0
3	ZN	B	1155	1/1	1.00	0.05	16,16,16,16	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.

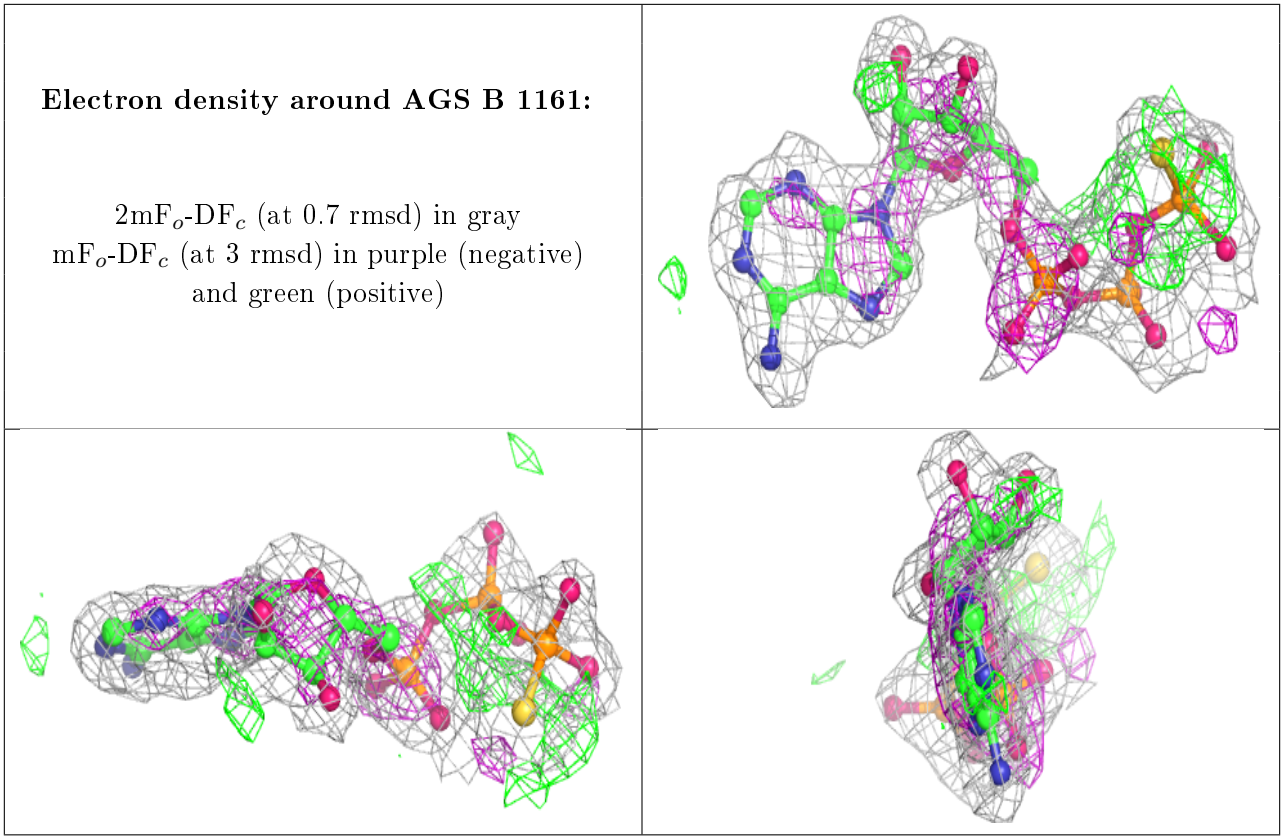
Electron density around AGS A 1162:

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



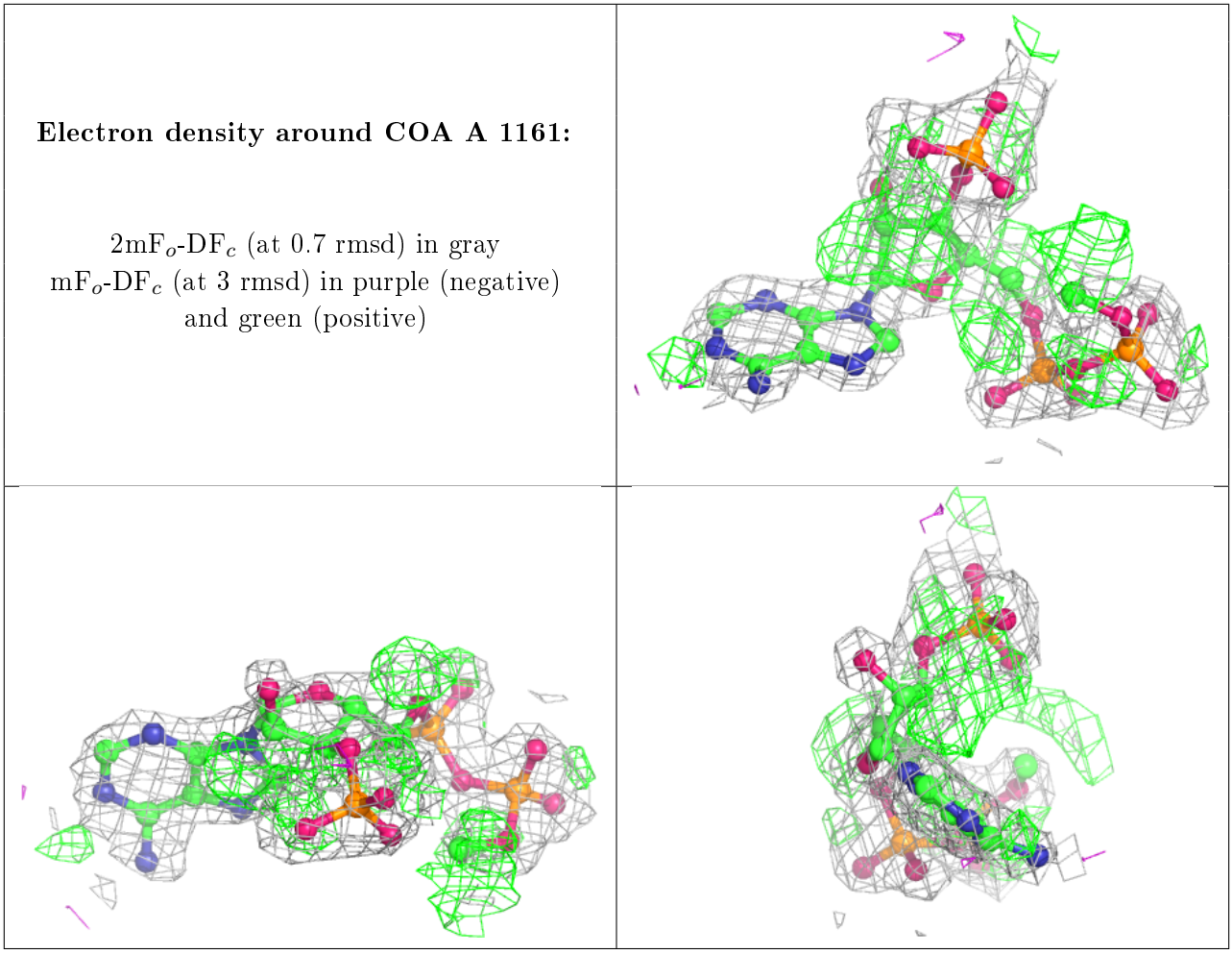
Electron density around AGS B 1161:

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



Electron density around COA A 1161:

$2mF_o$-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

There are no such residues in this entry.