



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:05 AM UTC

PDB ID : 2QF7 / pdb_00002qf7
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 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

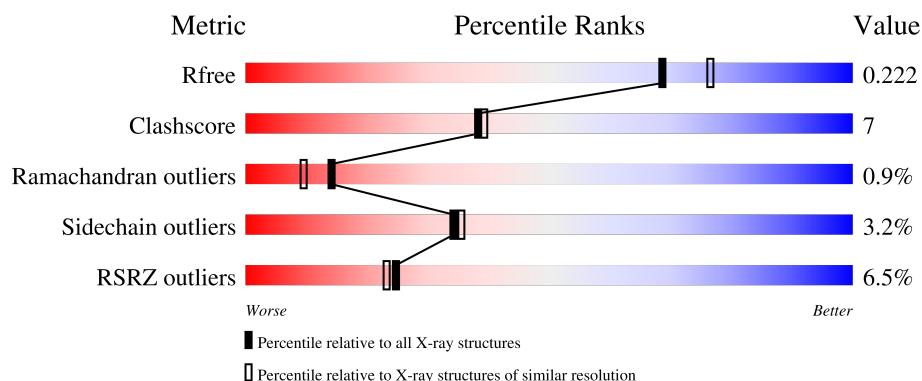
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	1165	6% 78% 12% 8%
1	B	1165	6% 78% 9% 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

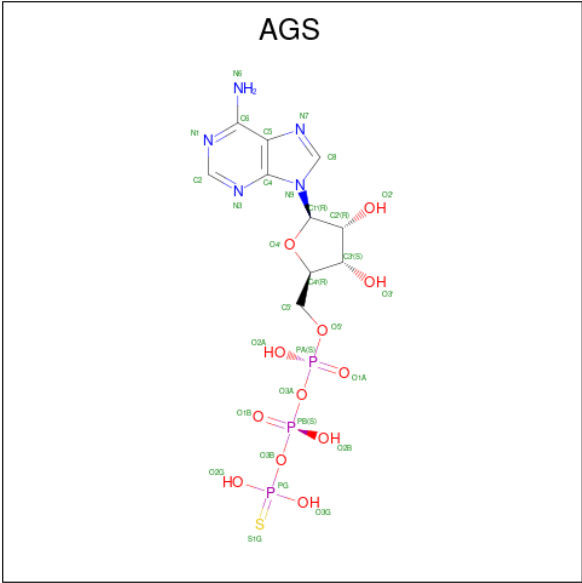
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	B	2	Total 2	Cl 2	0	0

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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 (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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 (CCD ID: FMT) (formula: CH_2O_2).



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

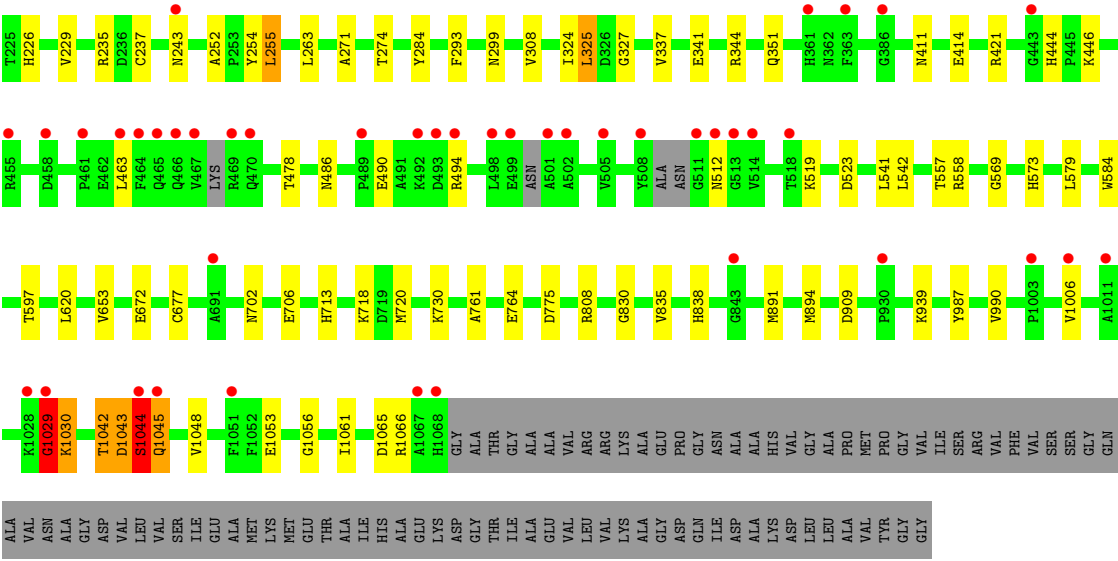
- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 9 is water.

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



4 Data and refinement statistics

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 – 2.00 130.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (131.31-2.00) 96.9 (130.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.88%)	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 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, GOL, KCX, AGS, MG, ZN, FMT, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	3/8518 (0.0%)	1.02	30/11577 (0.3%)
1	B	0.93	2/8107 (0.0%)	0.96	11/11005 (0.1%)
All	All	0.95	5/16625 (0.0%)	0.99	41/22582 (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
1	A	0	5
1	B	0	4
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	VAL	CA-CB	6.96	1.59	1.54
1	A	1124	ILE	CA-CB	6.69	1.61	1.54
1	B	1006	VAL	CA-CB	6.18	1.61	1.54
1	A	302	ILE	CA-CB	5.89	1.59	1.54
1	A	715	ILE	CA-CB	5.13	1.60	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1139	ALA	N-CA-C	12.50	129.78	109.40
1	A	1084	ALA	N-CA-C	9.14	125.12	113.88
1	B	163	VAL	N-CA-C	9.02	123.19	109.20
1	A	882[A]	THR	CA-C-N	7.23	131.47	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882[A]	THR	C-N-CA	7.23	131.47	123.73
1	A	882[B]	THR	CA-C-N	7.23	131.47	123.73
1	A	882[B]	THR	C-N-CA	7.23	131.47	123.73
1	B	126	ALA	N-CA-C	-6.87	103.88	111.36
1	A	1075	VAL	N-CA-C	6.71	123.29	109.34
1	A	1084	ALA	CA-C-N	6.39	133.20	121.70
1	A	1084	ALA	C-N-CA	6.39	133.20	121.70
1	B	830	GLY	CA-C-N	6.36	126.33	119.78
1	B	830	GLY	C-N-CA	6.36	126.33	119.78
1	B	243	ASN	N-CA-C	6.33	120.31	112.47
1	B	1044	SER	N-CA-C	-6.26	97.46	110.80
1	A	1105	ALA	N-CA-C	6.07	123.74	110.80
1	A	1083	ASN	N-CA-C	6.03	119.38	110.46
1	A	958	GLU	N-CA-C	-5.96	99.69	109.40
1	A	653	VAL	CB-CA-C	-5.83	102.91	110.84
1	B	145	LEU	N-CA-C	5.73	122.47	109.81
1	A	1077	ARG	CA-C-N	5.59	131.75	121.70
1	A	1077	ARG	C-N-CA	5.59	131.75	121.70
1	A	507	PRO	CA-C-N	-5.58	115.02	122.72
1	A	507	PRO	C-N-CA	-5.58	115.02	122.72
1	A	1122	THR	CA-C-N	5.42	131.45	121.70
1	A	1122	THR	C-N-CA	5.42	131.45	121.70
1	A	1138	LYS	CA-C-N	-5.30	114.98	122.94
1	A	1138	LYS	C-N-CA	-5.30	114.98	122.94
1	A	830	GLY	CA-C-N	5.28	125.22	119.78
1	A	830	GLY	C-N-CA	5.28	125.22	119.78
1	A	1103	GLY	N-CA-C	5.26	125.65	113.18
1	B	55	GLY	CA-C-N	5.25	126.41	119.84
1	B	55	GLY	C-N-CA	5.25	126.41	119.84
1	B	1029	GLY	N-CA-C	-5.23	100.78	113.18
1	A	55	GLY	CA-C-N	5.17	124.78	119.56
1	A	55	GLY	C-N-CA	5.17	124.78	119.56
1	A	252	ALA	CA-C-N	-5.16	114.35	119.56
1	A	252	ALA	C-N-CA	-5.16	114.35	119.56
1	A	53	GLY	N-CA-C	5.07	122.31	115.32
1	A	1102	SER	N-CA-C	5.04	121.53	110.80
1	B	1045	GLN	N-CA-C	-5.00	105.91	113.51

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

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	8123	140	0
1	B	7896	0	7704	83	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
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	15872	223	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 (223) 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:511:GLY:HA2	1:A:512:ASN:HB2	1.33	1.09
1:A:1095:ILE:HG12	1:A:1139:ALA:HB3	1.28	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:210:LEU:CB	1:A:211:VAL:HA	1.90	0.99
1:A:95:GLU:C	1:A:118[A]:MET:HE1	1.87	0.99
1:A:511:GLY:HA2	1:A:512:ASN:CB	1.95	0.97
1:A:1084:ALA:N	1:A:1085:ALA:HB3	1.79	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:HD22	1:A:500:ASN:N	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:95:GLU:O	1:A:118[A]:MET:HE1	1.75	0.87
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
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:1090:PRO:HG2	1:A:1091:MET:HE2	1.65	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:891[B]:MET:HE2	1:A:918:VAL:HG21	1.67	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:B:891:MET:HE1	1:B:894:MET:HE2	1.70	0.72
1:A:1138:LYS:CB	1:A:1141:ASP:OD2	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:891:MET:CE	1:B:894:MET:HE2	2.24	0.67
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:A:891[B]:MET:HE1	1:A:914:PHE:HD1	1.58	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:H	1:A:1083:ASN:HD22	1.45	0.64
1:B:130:LEU:HD21	1:B:274:THR:CG2	2.28	0.64
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:121:LEU:HD21	1:A:274:THR:HG21	1.78	0.63
1:A:1097:ARG:HD2	1:A:1099:PHE:CZ	2.34	0.63
1:A:444:HIS:CD2	1:A:446:LYS:H	2.17	0.62
1:A:1135:VAL:HG12	1:A:1137:VAL:O	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:164:MET:HE2	1:B:178:VAL:HG22	1.83	0.59
1:A:891[B]:MET:HE1	1:A:914:PHE:CD1	2.38	0.59
1:B:229:VAL:HG11	1:B:271:ALA:CB	2.32	0.59
1:A:511:GLY:HA2	1:A:512:ASN:CG	2.27	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: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: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:1084:ALA:H	1:A:1085:ALA:CB	2.19	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
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:B:891:MET:HE1	1:B:894:MET:CE	2.38	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:621[C]:ARG:CD	1:A:623:ALA:H	2.24	0.51
1:A:1145:ALA:O	1:A:1146:LYS:HB2	2.11	0.51
1:B:702:ASN:O	1:B:706[A]:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:GLU:O	1:A:118[A]:MET:CE	2.55	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:54:ARG:HD3	1:A:61:ASP:CG	2.39	0.46
1:A:421:ARG:HD2	1:A:421:ARG:C	2.40	0.46
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
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:677:CYS:N	1:A:713:HIS:HD2	2.09	0.46
1:A:118[A]:MET:HB3	1:A:118[A]:MET:HE2	1.32	0.46
1:B:164:MET:HB2	1:B:164:MET:HE3	1.70	0.46
1:A:470:GLN:HB2	5:A:1161:COA:O2A	2.16	0.45
1:A:461:PRO:HD2	9:A:1786:HOH:O	2.15	0.45
1:A:1122:THR:CA	1:A:1123:ALA:HB3	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1022[A]:LEU:C	1:A:1022[A]:LEU:HD12	2.43	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:57:HIS:HE1	1:B:73:GLU:CD	2.27	0.43
1:B:221:ILE:HD13	1:B:271:ALA:HB2	1.99	0.43
1:B:162:PRO:O	1:B:210:LEU:N	2.49	0.43
1:A:499:GLU:O	1:A:500:ASN:C	2.62	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: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:HB3	1:A:1110:ASP:CG	2.44	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:621[B]:ARG:CZ	1:A:621[B]:ARG:HB3	2.50	0.42
1:A:1016:LEU:HD21	1:A:1022[A]:LEU:HD23	2.01	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: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:254:TYR:CD1	1:B:255:LEU:HD13	2.55	0.41
1:B:891:MET:HE3	1:B:894:MET:HE2	2.03	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:621[C]:ARG:HH22	1:A:656:CYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:GLY:HA2	1:A:1131:THR:HA	2.03	0.41
1:B:263[A]:LEU:HD21	1:B:293:PHE:CD1	2.56	0.41
1:B:411[B]:ASN:HD21	1:B:414:GLU:H	1.66	0.40
1:B:1029:GLY:CA	1:B:1030:LYS:HB2	2.51	0.40
1:A:88:PRO:HG3	1:A:110:PHE:CZ	2.56	0.40
1:A:1022[B]:LEU:C	1:A:1022[B]:LEU:HD23	2.46	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:B:421:ARG:C	1:B:421:ARG:HD2	2.47	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%)	11	7
1	B	1032/1165 (89%)	1001 (97%)	24 (2%)	7 (1%)	18	14
All	All	2128/2330 (91%)	2056 (97%)	53 (2%)	19 (1%)	14	9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	512	ASN
1	A	1138	LYS

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Mol	Chain	Res	Type
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 ⓘ

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%)	807 (96%)	36 (4%)	26	25
1	B	803/934 (86%)	784 (98%)	19 (2%)	43	47
All	All	1646/1868 (88%)	1591 (97%)	55 (3%)	34	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	114	LYS
1	A	116	ASP
1	A	209	LYS
1	A	210	LEU
1	A	285	LEU
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	350	LEU
1	A	360	GLU
1	A	401	LEU
1	A	485	VAL
1	A	500	ASN
1	A	514	VAL
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	797	GLU
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	1135	VAL
1	A	1143	ILE
1	B	41	LEU
1	B	120	GLN
1	B	142	THR
1	B	145	LEU
1	B	255	LEU
1	B	299	ASN
1	B	325[A]	LEU
1	B	325[B]	LEU
1	B	344	ARG
1	B	463[A]	LEU
1	B	463[B]	LEU
1	B	542	LEU
1	B	557	THR

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Mol	Chain	Res	Type
1	B	584	TRP
1	B	597	THR
1	B	720	MET
1	B	775	ASP
1	B	939	LYS
1	B	1042	THR

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

Mol	Chain	Res	Type
1	A	23	ASN
1	A	129	ASN
1	A	226	HIS
1	A	243	ASN
1	A	275	ASN
1	A	334	GLN
1	A	348	HIS
1	A	351	GLN
1	A	444	HIS
1	A	500	ASN
1	A	642	GLN
1	A	713	HIS
1	A	820	GLN
1	A	863	GLN
1	A	873	GLN
1	A	898	GLN
1	A	928	GLN
1	A	1037	GLN
1	A	1045	GLN
1	A	1083	ASN
1	B	57	HIS
1	B	220	GLN
1	B	226	HIS
1	B	348	HIS
1	B	444	HIS
1	B	486	ASN
1	B	536	ASN
1	B	573	HIS
1	B	642	GLN
1	B	713	HIS
1	B	820	GLN
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 ⓘ

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	10,11,12	2.01	2 (20%)	6,12,14	4.34	1 (16%)
1	KCX	B	718[A]	1,3	10,11,12	1.66	1 (10%)	6,12,14	4.03	2 (33%)

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	-	1/9/10/12	-
1	KCX	B	718[A]	1,3	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718[A]	KCX	OQ1-CX	5.48	1.31	1.21
1	B	718[A]	KCX	OQ1-CX	4.53	1.30	1.21
1	A	718[A]	KCX	CE-NZ	2.25	1.51	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718[A]	KCX	OQ1-CX-NZ	-10.52	108.94	124.92
1	B	718[A]	KCX	OQ1-CX-NZ	-8.71	111.69	124.92
1	B	718[A]	KCX	CE-NZ-CX	4.25	129.20	121.98

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 oligosaccharides 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	$\# Z > 2$
6	AGS	A	1162	2	32,33,33	2.60	8 (25%)	45,52,52	1.83	11 (24%)
8	GOL	B	1162	-	5,5,5	0.29	0	5,5,5	0.69	0
7	FMT	B	1163	-	2,2,2	0.56	0	1,1,1	0.50	0
7	FMT	A	1163	-	2,2,2	0.79	0	1,1,1	0.30	0
6	AGS	B	1161	2	32,33,33	2.46	8 (25%)	45,52,52	1.85	10 (22%)
5	COA	A	1161	-	34,34,50	1.06	2 (5%)	50,53,75	1.87	12 (24%)

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	COA	A	1161	-	-	6/24/40/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGS	A	1162	2	-	9/21/38/38	0/3/3/3
8	GOL	B	1162	-	-	2/4/4/4	-
6	AGS	B	1161	2	-	4/21/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1162	AGS	PG-O2G	7.48	1.79	1.54
6	A	1162	AGS	PG-O3G	7.38	1.78	1.54
6	B	1161	AGS	PG-O2G	7.36	1.78	1.54
6	B	1161	AGS	PG-O3G	6.99	1.77	1.54
6	B	1161	AGS	C5-C4	5.77	1.49	1.39
6	A	1162	AGS	C5-C4	5.71	1.49	1.39
6	A	1162	AGS	PA-O3A	4.35	1.64	1.59
6	A	1162	AGS	C8-N7	3.23	1.37	1.31
6	A	1162	AGS	C5-C6	3.14	1.49	1.41
6	A	1162	AGS	PB-O3A	3.02	1.62	1.59
6	B	1161	AGS	C8-N7	2.98	1.37	1.31
6	B	1161	AGS	PA-O3A	2.80	1.62	1.59
5	A	1161	COA	C2A-N3A	2.62	1.38	1.33
6	B	1161	AGS	PG-S1G	2.57	1.96	1.90
6	B	1161	AGS	C5-C6	2.56	1.48	1.41
5	A	1161	COA	C2A-N1A	2.51	1.38	1.33
6	A	1162	AGS	PG-S1G	2.38	1.95	1.90
6	B	1161	AGS	C4-N3	2.07	1.38	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1161	COA	N3A-C2A-N1A	-6.07	119.39	128.58
6	A	1162	AGS	C5-C4-N3	-5.58	119.03	126.72
5	A	1161	COA	C5A-C4A-N3A	-5.10	119.69	126.72
6	B	1161	AGS	C5-C4-N3	-4.85	120.05	126.72
6	B	1161	AGS	N3-C4-N9	4.60	134.99	127.17
6	A	1162	AGS	N3-C4-N9	4.20	134.31	127.17
5	A	1161	COA	C2A-N3A-C4A	3.81	121.14	111.83
5	A	1161	COA	N9A-C8A-N7A	-3.77	108.59	113.94
6	B	1161	AGS	N3-C2-N1	-3.75	122.91	128.58
5	A	1161	COA	N3A-C4A-N9A	3.63	133.34	127.17
6	A	1162	AGS	C2-N3-C4	3.54	120.48	111.83
6	A	1162	AGS	N3-C2-N1	-3.42	123.40	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1161	COA	C5A-N7A-C8A	3.40	108.79	103.45
6	A	1162	AGS	C4-C5-N7	-3.29	106.81	110.58
6	B	1161	AGS	C2-N3-C4	3.20	119.64	111.83
6	B	1161	AGS	C4-N9-C8	3.04	108.93	105.74
6	A	1162	AGS	PB-O3B-PG	-2.97	122.30	133.17
6	B	1161	AGS	O2G-PG-O3B	2.97	114.54	104.64
5	A	1161	COA	P3B-O3B-C3B	-2.95	115.56	123.43
6	B	1161	AGS	C2-N1-C6	2.74	123.24	118.73
5	A	1161	COA	C5B-C4B-C3B	-2.67	105.47	114.38
6	B	1161	AGS	N6-C6-N1	2.57	124.09	118.38
6	A	1162	AGS	O2G-PG-O3B	2.55	113.14	104.64
6	B	1161	AGS	O2A-PA-O3A	2.39	113.74	107.27
5	A	1161	COA	C5A-C6A-N6A	-2.37	117.42	123.29
6	A	1162	AGS	O4'-C1'-N9	2.35	112.59	108.09
6	A	1162	AGS	C2-N1-C6	2.30	122.50	118.73
6	B	1161	AGS	O2B-PB-O3B	2.28	113.43	107.27
5	A	1161	COA	O5A-P2A-O3A	2.11	112.98	107.27
6	A	1162	AGS	C6-C5-N7	2.11	136.16	132.09
6	A	1162	AGS	C5-N7-C8	2.11	106.76	103.45
5	A	1161	COA	C6A-C5A-C4A	2.09	120.03	117.18
5	A	1161	COA	O3A-P1A-O1A	-2.07	104.48	110.70

There are no chirality outliers.

All (21) 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	C5'-O5'-PA-O3A
6	A	1162	AGS	O4'-C4'-C5'-O5'
6	B	1161	AGS	PB-O3B-PG-O2G
6	A	1162	AGS	C3'-C4'-C5'-O5'
5	A	1161	COA	CCP-O6A-P2A-O4A
8	B	1162	GOL	C1-C2-C3-O3
6	A	1162	AGS	PB-O3A-PA-O2A
6	B	1161	AGS	PB-O3A-PA-O2A
5	A	1161	COA	C5B-O5B-P1A-O1A
8	B	1162	GOL	O2-C2-C3-O3
5	A	1161	COA	CCP-O6A-P2A-O5A
5	A	1161	COA	CCP-O6A-P2A-O3A
6	B	1161	AGS	PB-O3A-PA-O1A

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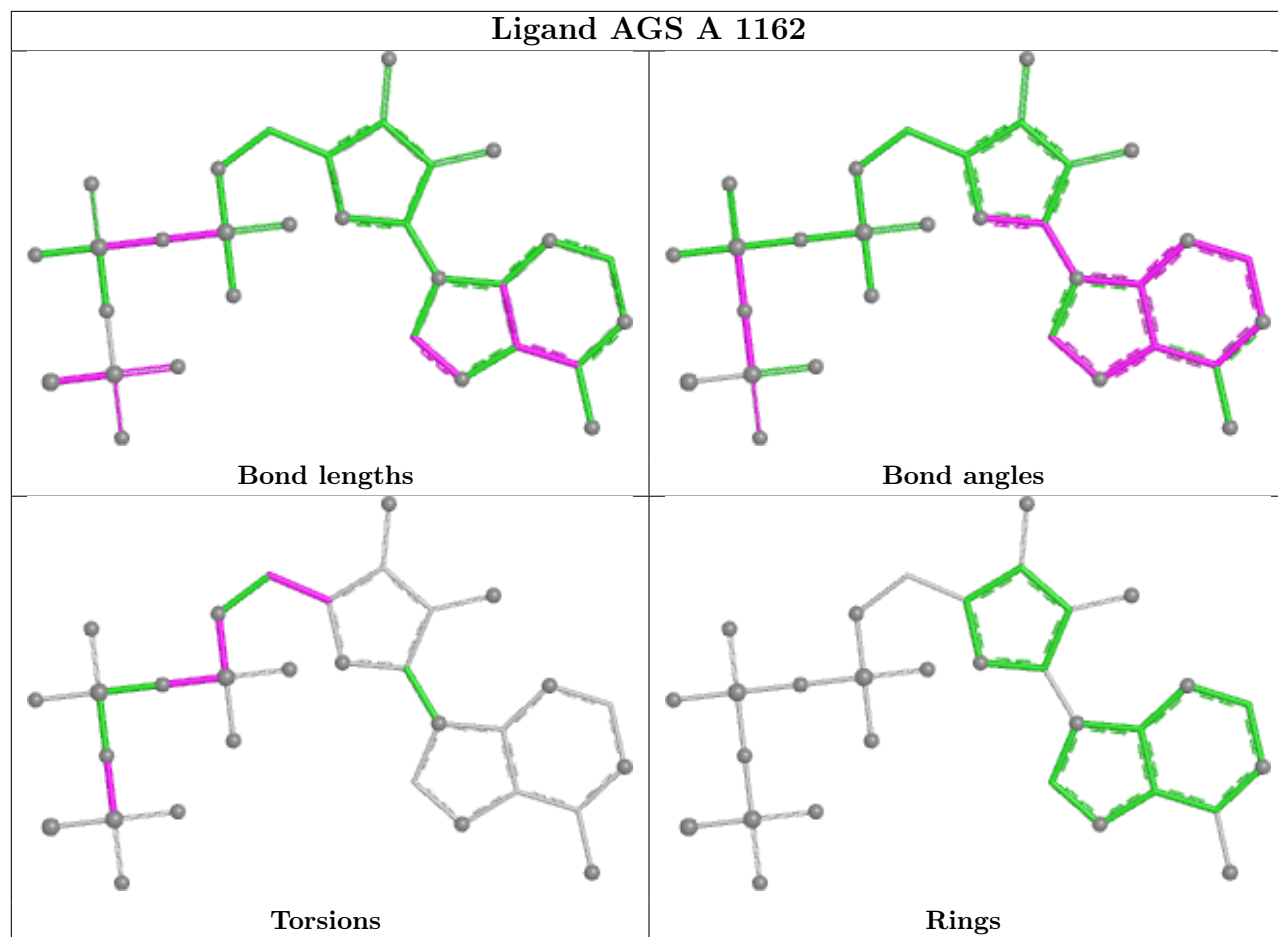
Mol	Chain	Res	Type	Atoms
6	A	1162	AGS	PB-O3B-PG-O3G
6	B	1161	AGS	O4'-C4'-C5'-O5'
5	A	1161	COA	P1A-O3A-P2A-O4A
5	A	1161	COA	P1A-O3A-P2A-O5A
6	A	1162	AGS	PB-O3A-PA-O1A

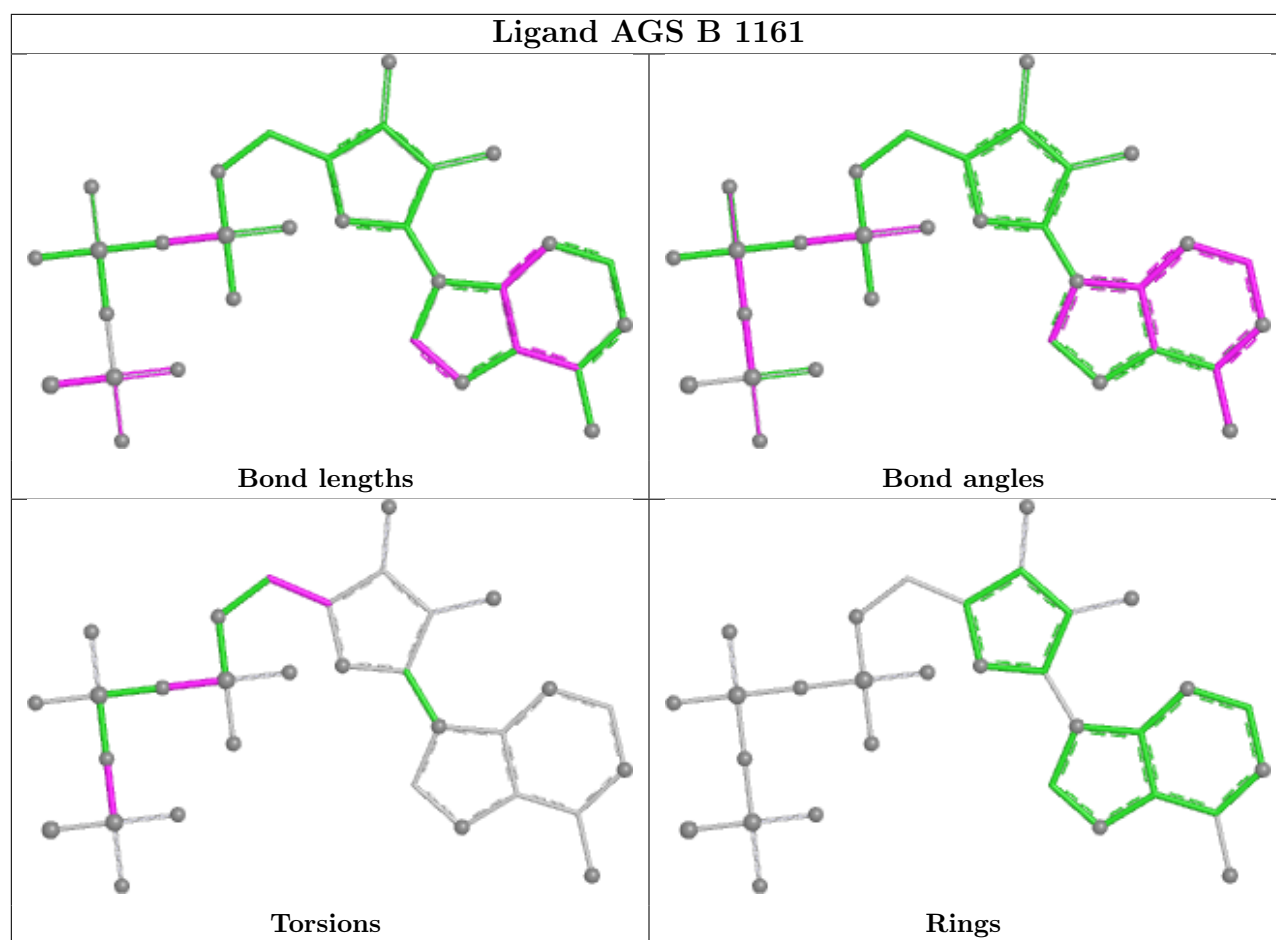
There are no ring outliers.

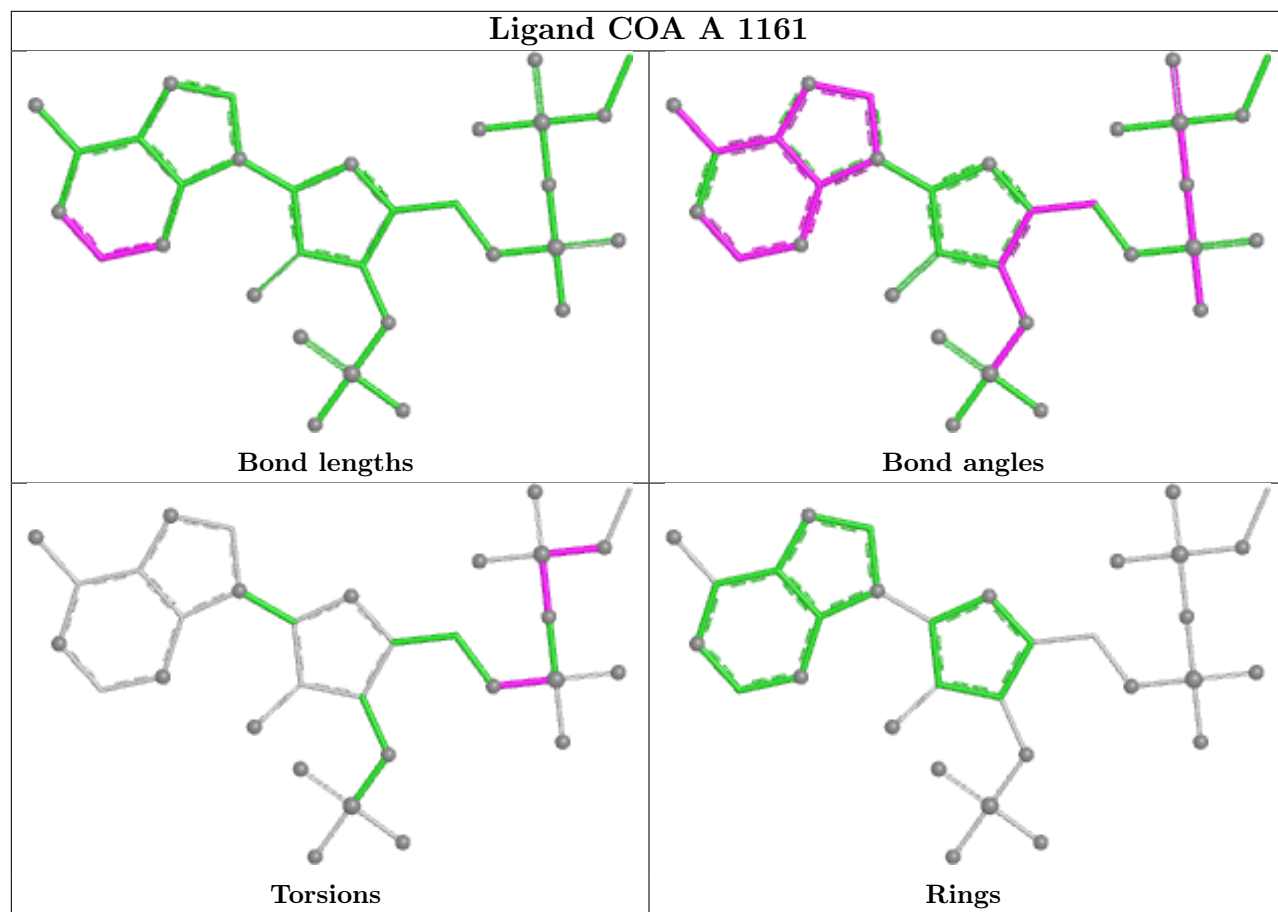
1 monomer is involved in 4 short contacts:

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 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	1075/1165 (92%)	0.43	66 (6%) 27 26	7, 24, 37, 52	43 (4%)
1	B	1016/1165 (87%)	0.46	70 (6%) 23 21	10, 24, 39, 64	40 (3%)
All	All	2091/2330 (89%)	0.45	136 (6%) 25 23	7, 24, 38, 64	83 (3%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	LYS	8.2
1	A	509	ALA	8.0
1	A	1075	VAL	7.7
1	B	207	LEU	7.3
1	B	162	PRO	5.7
1	A	508	TYR	5.6
1	A	467	VAL	5.5
1	A	512	ASN	5.5
1	B	146	PRO	5.5
1	A	502	ALA	5.0
1	A	1077	ARG	5.0
1	B	142	THR	4.8
1	A	501	ALA	4.8
1	B	513	GLY	4.8
1	B	511	GLY	4.7
1	B	56	PRO	4.7
1	B	512	ASN	4.6
1	B	467	VAL	4.6
1	A	1081	PRO	4.5
1	B	499	GLU	4.4
1	B	144	PRO	4.3
1	B	164	MET	4.2
1	B	508	TYR	4.2
1	A	210	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1071	THR	4.1
1	B	843	GLY	4.0
1	A	511	GLY	4.0
1	B	145	LEU	4.0
1	B	501	ALA	4.0
1	A	1078	LYS	4.0
1	B	176	MET	4.0
1	A	123	ASN	3.9
1	A	492	LYS	3.9
1	A	1074	ALA	3.9
1	A	498	LEU	3.9
1	A	243	ASN	3.8
1	A	1076	ARG	3.8
1	B	178	VAL	3.8
1	A	500	ASN	3.7
1	B	461	PRO	3.7
1	B	141	ALA	3.7
1	B	165	LEU	3.6
1	A	1117	ALA	3.6
1	A	1070	ALA	3.6
1	B	1044	SER	3.6
1	B	470	GLN	3.6
1	B	493	ASP	3.6
1	B	458	ASP	3.5
1	B	179	ILE	3.5
1	A	461	PRO	3.5
1	B	1068	HIS	3.5
1	A	470	GLN	3.5
1	A	468	LYS	3.5
1	B	58	LEU	3.5
1	A	513	GLY	3.4
1	B	163	VAL	3.4
1	A	466	GLN	3.3
1	A	1084	ALA	3.3
1	A	363	PHE	3.3
1	A	957	LYS	3.3
1	A	1102	SER	3.2
1	B	180	ARG	3.2
1	B	465	GLN	3.2
1	B	167	ALA	3.1
1	A	1082	GLY	3.1
1	B	386	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLU	3.0
1	A	621[A]	ARG	3.0
1	A	130	LEU	3.0
1	B	691	ALA	2.9
1	B	57	HIS	2.9
1	A	1106	VAL	2.9
1	B	125	VAL	2.9
1	A	242	ARG	2.9
1	B	1051[A]	PHE	2.9
1	A	1100	VAL	2.8
1	A	1080	GLU	2.8
1	B	123	ASN	2.8
1	B	494	ARG	2.8
1	A	1137	VAL	2.8
1	A	464	PHE	2.8
1	B	464	PHE	2.8
1	B	1029	GLY	2.8
1	B	469	ARG	2.7
1	A	456	PHE	2.7
1	A	1134	GLU	2.7
1	A	1	GLY	2.6
1	B	502	ALA	2.6
1	B	168	SER	2.6
1	A	465	GLN	2.6
1	B	1045	GLN	2.6
1	A	469	ARG	2.6
1	B	455	ARG	2.6
1	B	1067	ALA	2.5
1	A	691	ALA	2.5
1	B	1006	VAL	2.5
1	B	243	ASN	2.5
1	A	1072	GLY	2.5
1	B	206	TYR	2.4
1	A	1079	ALA	2.4
1	A	362	ASN	2.4
1	B	466	GLN	2.4
1	A	211	VAL	2.4
1	B	361	HIS	2.4
1	B	463[A]	LEU	2.3
1	A	1140	GLY	2.3
1	A	1110	ASP	2.3
1	A	496	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1028	LYS	2.3
1	B	498	LEU	2.3
1	A	503	ARG	2.3
1	A	931	SER	2.3
1	A	1138	LYS	2.3
1	B	930	PRO	2.3
1	A	1105	ALA	2.3
1	B	55	GLY	2.3
1	B	489	PRO	2.2
1	A	962	ASP	2.2
1	A	1073	ALA	2.2
1	A	139	VAL	2.2
1	B	205	VAL	2.2
1	B	505	VAL	2.2
1	B	1003	PRO	2.1
1	B	514	VAL	2.1
1	B	124	LYS	2.1
1	A	495	PRO	2.1
1	A	240	GLN	2.1
1	A	57	HIS	2.1
1	B	492	LYS	2.1
1	B	363	PHE	2.1
1	A	1127	GLU	2.0
1	B	1011	ALA	2.1
1	B	518	THR	2.0
1	B	443	GLY	2.0
1	A	1139	ALA	2.0
1	B	60	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	KCX	A	718[A]	12/13	0.92	0.10	21,23,25,27	0
1	KCX	B	718[A]	12/13	0.94	0.08	21,23,28,29	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

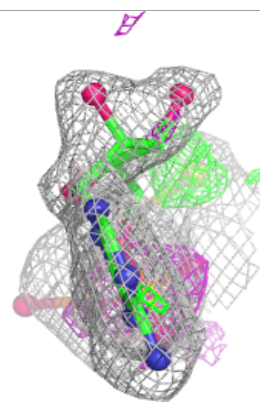
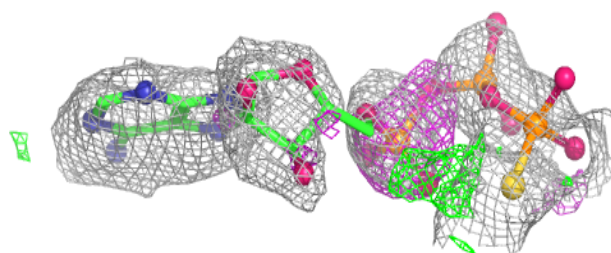
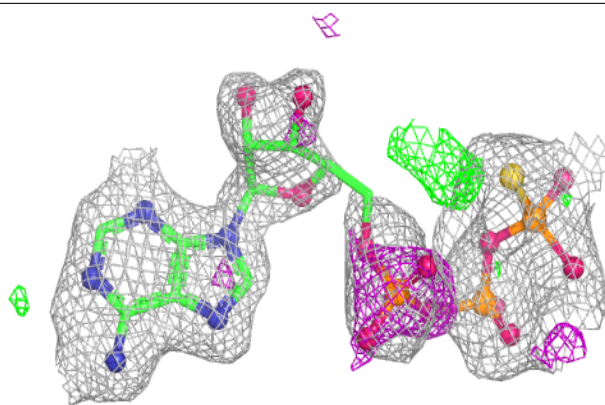
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AGS	A	1162	31/31	0.73	0.18	36,48,50,52	12
6	AGS	B	1161	31/31	0.76	0.17	24,39,43,44	9
8	GOL	B	1162	6/6	0.85	0.18	30,34,39,46	0
5	COA	A	1161	32/48	0.87	0.15	16,20,25,27	32
2	MG	A	1156	1/1	0.87	0.14	39,39,39,39	0
2	MG	B	1158	1/1	0.93	0.17	24,24,24,24	0
2	MG	B	1157	1/1	0.94	0.14	34,34,34,34	0
4	CL	B	1160	1/1	0.95	0.13	38,38,38,38	0
7	FMT	A	1163	3/3	0.96	0.15	18,18,19,19	0
7	FMT	B	1163	3/3	0.97	0.16	18,18,18,19	0
2	MG	A	1158	1/1	0.97	0.22	17,17,17,17	0
4	CL	B	1159	1/1	0.98	0.14	28,28,28,28	0
2	MG	A	1155	1/1	0.98	0.05	13,13,13,13	1
4	CL	A	1159	1/1	0.98	0.20	24,24,24,24	0
4	CL	A	1160	1/1	0.98	0.17	35,35,35,35	0
2	MG	B	1156	1/1	0.99	0.07	20,20,20,20	0
3	ZN	A	1157	1/1	0.99	0.14	15,15,15,15	0
3	ZN	B	1155	1/1	1.00	0.12	16,16,16,16	0

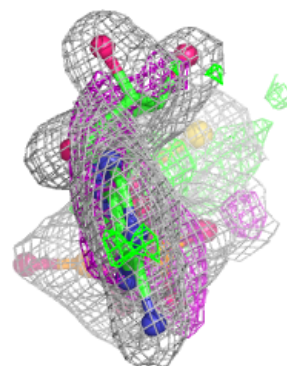
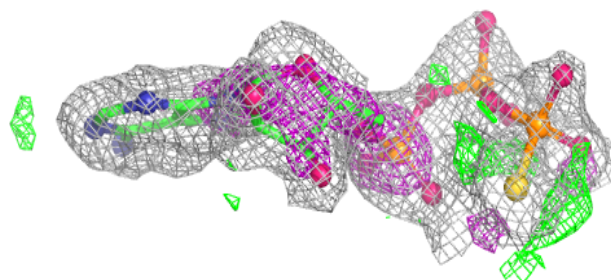
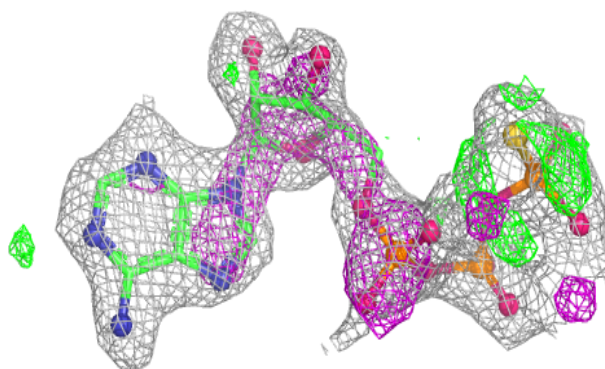
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

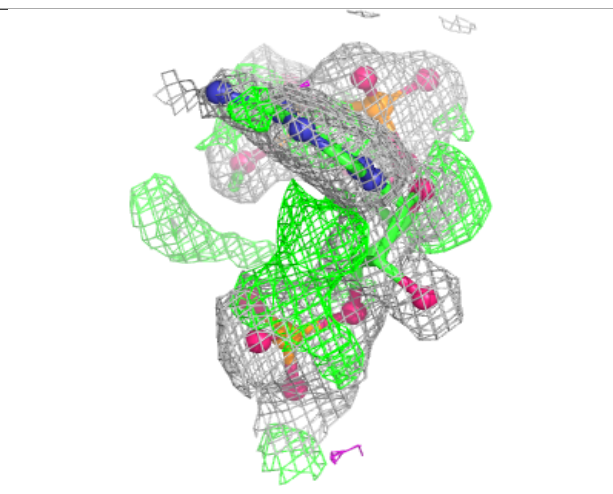
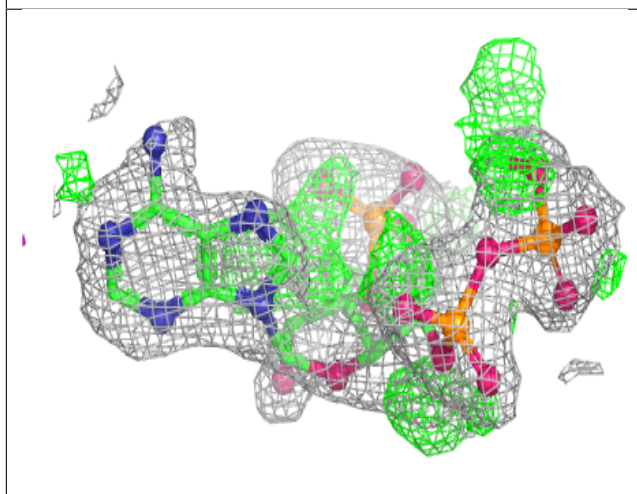
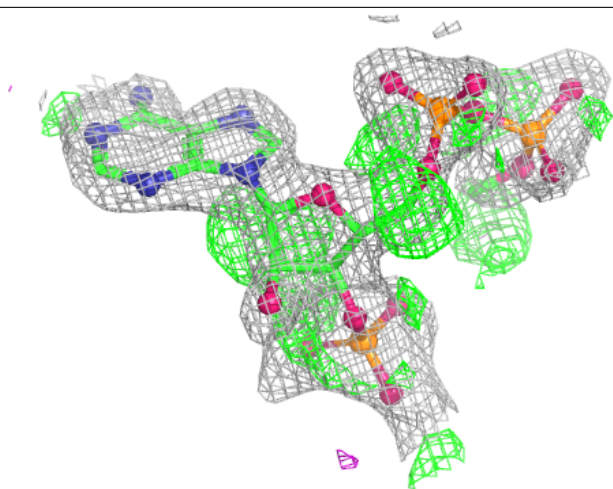
**Electron density around AGS B 1161:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.