



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 03:30 AM EDT

PDB ID : 5VXD
Title : Crystal structure of Xanthomonas campestris OleA E117A
Authors : Jensen, M.R.; Wilmot, C.M.
Deposited on : 2017-05-23
Resolution : 1.97 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

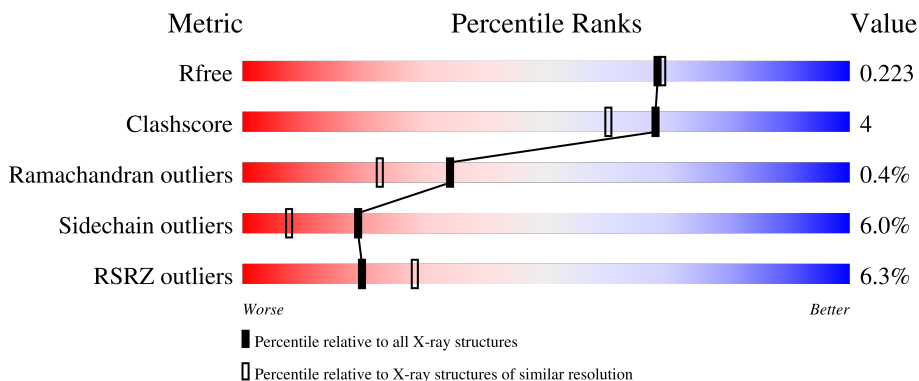
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	358	 3% 81% 13% • •
1	B	358	 9% 77% 16% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5431 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 3-oxoacyl-[ACP] synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	2641	1658	467	500	16	0	3	0
1	B	340	2600	1631	459	494	16	0	3	0

There are 42 discrepancies between the modelled and reference sequences:

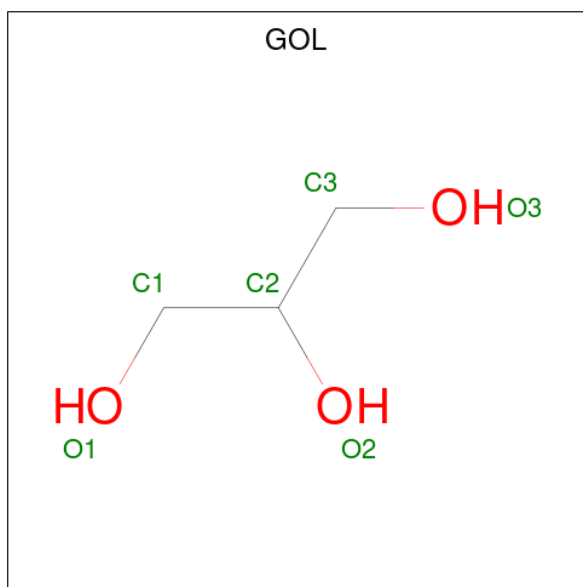
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8PDX2
A	2	GLY	-	expression tag	UNP Q8PDX2
A	3	SER	-	expression tag	UNP Q8PDX2
A	4	SER	-	expression tag	UNP Q8PDX2
A	5	HIS	-	expression tag	UNP Q8PDX2
A	6	HIS	-	expression tag	UNP Q8PDX2
A	7	HIS	-	expression tag	UNP Q8PDX2
A	8	HIS	-	expression tag	UNP Q8PDX2
A	9	HIS	-	expression tag	UNP Q8PDX2
A	10	HIS	-	expression tag	UNP Q8PDX2
A	11	SER	-	expression tag	UNP Q8PDX2
A	12	SER	-	expression tag	UNP Q8PDX2
A	13	GLY	-	expression tag	UNP Q8PDX2
A	14	LEU	-	expression tag	UNP Q8PDX2
A	15	VAL	-	expression tag	UNP Q8PDX2
A	16	PRO	-	expression tag	UNP Q8PDX2
A	17	ARG	-	expression tag	UNP Q8PDX2
A	18	GLY	-	expression tag	UNP Q8PDX2
A	19	SER	-	expression tag	UNP Q8PDX2
A	20	HIS	-	expression tag	UNP Q8PDX2
A	117	ALA	GLU	engineered mutation	UNP Q8PDX2
B	1	MET	-	initiating methionine	UNP Q8PDX2
B	2	GLY	-	expression tag	UNP Q8PDX2
B	3	SER	-	expression tag	UNP Q8PDX2
B	4	SER	-	expression tag	UNP Q8PDX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP Q8PDX2
B	6	HIS	-	expression tag	UNP Q8PDX2
B	7	HIS	-	expression tag	UNP Q8PDX2
B	8	HIS	-	expression tag	UNP Q8PDX2
B	9	HIS	-	expression tag	UNP Q8PDX2
B	10	HIS	-	expression tag	UNP Q8PDX2
B	11	SER	-	expression tag	UNP Q8PDX2
B	12	SER	-	expression tag	UNP Q8PDX2
B	13	GLY	-	expression tag	UNP Q8PDX2
B	14	LEU	-	expression tag	UNP Q8PDX2
B	15	VAL	-	expression tag	UNP Q8PDX2
B	16	PRO	-	expression tag	UNP Q8PDX2
B	17	ARG	-	expression tag	UNP Q8PDX2
B	18	GLY	-	expression tag	UNP Q8PDX2
B	19	SER	-	expression tag	UNP Q8PDX2
B	20	HIS	-	expression tag	UNP Q8PDX2
B	117	ALA	GLU	engineered mutation	UNP Q8PDX2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

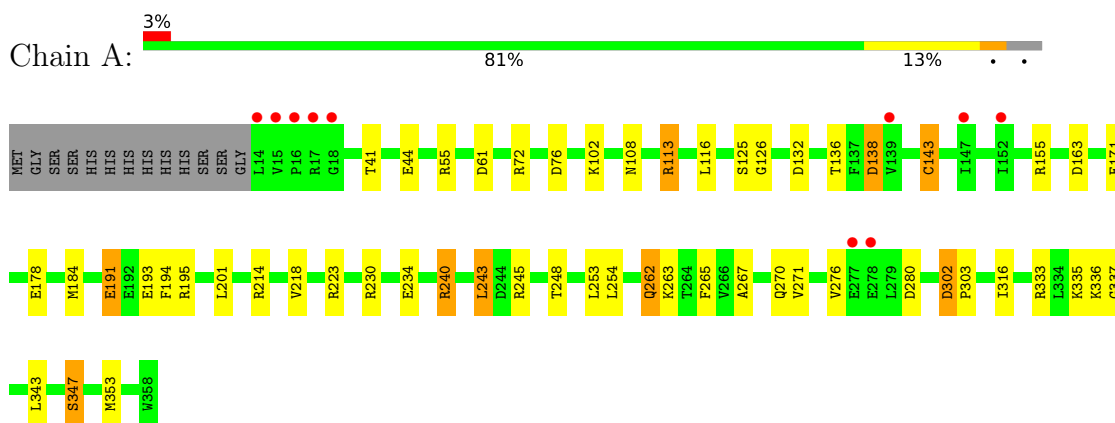
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total 106	O 106	0	0
3	B	72	Total 72	O 72	0	0

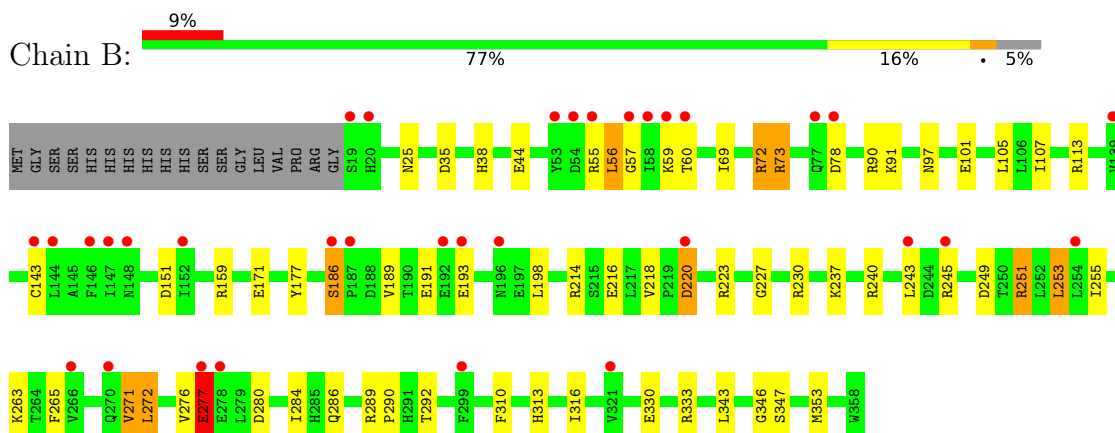
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 3-oxoacyl-[ACP] synthase III



- Molecule 1: 3-oxoacyl-[ACP] synthase III



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.39Å 85.99Å 103.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.97 32.04 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.97) 99.6 (32.04-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.169 , 0.214 0.179 , 0.223	Depositor DCC
R_{free} test set	2646 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtrriage
Anisotropy	0.123	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.024 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.39	13/2681 (0.5%)	1.30	24/3630 (0.7%)
1	B	1.30	9/2639 (0.3%)	1.30	22/3573 (0.6%)
All	All	1.34	22/5320 (0.4%)	1.30	46/7203 (0.6%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLU	CG-CD	11.37	1.69	1.51
1	A	347	SER	CB-OG	-10.11	1.29	1.42
1	A	178	GLU	CB-CG	9.74	1.70	1.52
1	A	333	ARG	CZ-NH2	8.19	1.43	1.33
1	B	44	GLU	CD-OE1	8.01	1.34	1.25
1	A	178	GLU	CD-OE2	6.72	1.33	1.25
1	A	178	GLU	CD-OE1	6.38	1.32	1.25
1	B	216	GLU	CD-OE1	6.30	1.32	1.25
1	B	347	SER	CB-OG	-5.97	1.34	1.42
1	B	44	GLU	CG-CD	5.92	1.60	1.51
1	B	101	GLU	CD-OE1	5.83	1.32	1.25
1	A	138	ASP	CG-OD2	5.80	1.38	1.25
1	A	193	GLU	CG-CD	5.65	1.60	1.51
1	B	44	GLU	CD-OE2	5.64	1.31	1.25
1	A	337	GLY	N-CA	-5.54	1.37	1.46
1	B	249	ASP	CB-CG	5.33	1.62	1.51
1	A	126	GLY	N-CA	5.22	1.53	1.46
1	B	78	ASP	CA-C	5.13	1.66	1.52
1	B	177	TYR	CZ-OH	-5.12	1.29	1.37
1	A	194	PHE	CB-CG	-5.12	1.42	1.51
1	A	193	GLU	CD-OE2	5.11	1.31	1.25
1	A	191	GLU	CB-CG	-5.04	1.42	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASP	CB-CG-OD2	-10.25	109.08	118.30
1	B	90	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	B	253	LEU	CA-CB-CG	9.34	136.78	115.30
1	A	55	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	B	214	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	B	159	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	A	240	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	302	ASP	CB-CG-OD1	8.72	126.15	118.30
1	B	159	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	B	223	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	223	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	249	ASP	CB-CG-OD1	7.82	125.34	118.30
1	B	113	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	155	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	132	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	151	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	230	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	178	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	B	72	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	163	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	230	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	113	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	333	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	A	113	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	B	353	MET	CG-SD-CE	-6.17	90.34	100.20
1	B	249	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	280	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	73	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	280	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	171	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	214	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	343	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	35	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	171	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	B	90	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	155	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	243	LEU	CB-CG-CD2	5.51	120.37	111.00
1	A	234	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	A	178	GLU	CB-CG-CD	5.37	128.69	114.20
1	A	55	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	245	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	76	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	61	ASP	CB-CG-OD1	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	347	SER	CB-CA-C	5.07	119.74	110.10
1	B	280	ASP	CB-CG-OD2	5.00	122.80	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	2641	0	2677	20	0
1	B	2600	0	2631	20	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	106	0	0	3	0
3	B	72	0	0	1	0
All	All	5431	0	5324	40	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 4.

All (40) 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:184:MET:HE1	1:A:201:LEU:HD11	1.25	1.10
1:A:143[A]:CYS:HB3	3:A:599:HOH:O	1.60	1.01
1:B:143[B]:CYS:SG	3:B:567:HOH:O	2.30	0.88
1:A:143[B]:CYS:SG	3:A:599:HOH:O	2.46	0.72
1:A:184:MET:HE1	1:A:201:LEU:CD1	2.13	0.71
1:A:41:THR:OG1	1:A:44[B]:GLU:HG3	1.91	0.69
1:A:184:MET:CE	1:A:201:LEU:HD11	2.15	0.67
1:B:56:LEU:HD13	1:B:191:GLU:HB2	1.80	0.64
1:B:25[A]:ASN:OD1	1:B:25[A]:ASN:N	2.31	0.64
1:B:220:ASP:OD1	1:B:220:ASP:N	2.28	0.61
1:B:191:GLU:O	1:B:191:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:HD11	1:B:292:THR:HG23	1.88	0.56
1:A:108:ASN:HB3	1:A:138:ASP:OD1	2.07	0.54
1:B:227:GLY:HA2	1:B:272:LEU:HD11	1.90	0.54
1:B:143[A]:CYS:SG	1:B:346:GLY:HA2	2.48	0.53
1:B:276:VAL:O	1:B:277:GLU:HB3	2.08	0.53
1:B:69:ILE:HB	1:B:310:PHE:CE2	2.44	0.52
1:B:191:GLU:O	1:B:191:GLU:CG	2.57	0.51
1:A:240:ARG:HD3	3:A:587:HOH:O	2.10	0.51
1:B:289:ARG:HB3	1:B:290:PRO:HD3	1.93	0.50
1:B:271:VAL:HG22	1:B:272:LEU:CD1	2.42	0.50
1:A:343:LEU:HD22	1:A:353:MET:HG2	1.93	0.48
1:B:271:VAL:HG22	1:B:272:LEU:HD13	1.94	0.48
1:A:262[A]:GLN:HG2	1:A:263:LYS:N	2.29	0.48
1:B:251:ARG:O	1:B:255:ILE:HD12	2.14	0.47
1:A:125:SER:OG	1:A:136:THR:HG21	2.16	0.46
1:A:218:VAL:O	1:A:218:VAL:HG23	2.16	0.46
1:B:105:LEU:HD21	1:B:107:ILE:HD11	1.98	0.45
1:A:254:LEU:C	1:A:254:LEU:HD23	2.38	0.44
1:B:218:VAL:HG23	1:B:218:VAL:O	2.19	0.43
1:B:313:HIS:HB3	1:B:316:ILE:HD11	2.01	0.42
1:A:113:ARG:NH1	1:A:116:LEU:CD2	2.83	0.42
1:B:186:SER:O	1:B:189:VAL:HG12	2.19	0.42
1:A:191:GLU:HG2	1:A:195:ARG:CZ	2.50	0.41
1:A:267:ALA:O	1:A:271:VAL:HG13	2.20	0.41
1:B:38:HIS:O	1:B:73:ARG:HA	2.21	0.41
1:A:316:ILE:HD13	1:A:316:ILE:HG21	1.87	0.40
1:A:248:THR:CG2	1:A:253:LEU:HD12	2.51	0.40
1:A:267:ALA:HA	1:A:270:GLN:HE21	1.86	0.40
1:A:302:ASP:HA	1:A:303:PRO:HD3	1.92	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	346/358 (97%)	336 (97%)	10 (3%)	0	100	100
1	B	341/358 (95%)	325 (95%)	13 (4%)	3 (1%)	17	8
All	All	687/716 (96%)	661 (96%)	23 (3%)	3 (0%)	34	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ARG
1	B	277	GLU
1	B	57	GLY

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	281/289 (97%)	269 (96%)	12 (4%)	29	16
1	B	277/289 (96%)	254 (92%)	23 (8%)	11	3
All	All	558/578 (96%)	523 (94%)	35 (6%)	19	7

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	102	LYS
1	A	143[A]	CYS
1	A	143[B]	CYS
1	A	243	LEU
1	A	262[A]	GLN
1	A	262[B]	GLN
1	A	265	PHE
1	A	276	VAL
1	A	335	LYS
1	A	336	LYS
1	A	347	SER
1	B	56	LEU

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Mol	Chain	Res	Type
1	B	59	LYS
1	B	60	THR
1	B	72	ARG
1	B	91	LYS
1	B	97	ASN
1	B	186	SER
1	B	193	GLU
1	B	198	LEU
1	B	220	ASP
1	B	237	LYS
1	B	240	ARG
1	B	243	LEU
1	B	245	ARG
1	B	251	ARG
1	B	253	LEU
1	B	263	LYS
1	B	265	PHE
1	B	271	VAL
1	B	272	LEU
1	B	277	GLU
1	B	286	GLN
1	B	330	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	B	270	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

2 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
2	GOL	A	401	-	5,5,5	0.28	0	5,5,5	1.26	1 (20%)
2	GOL	B	401	-	5,5,5	0.42	0	5,5,5	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GOL	O2-C2-C3	2.08	118.28	109.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	345/358 (96%)	-0.04	10 (2%) 51 60	18, 28, 46, 74	0
1	B	340/358 (94%)	0.43	33 (9%) 7 12	17, 31, 71, 98	0
All	All	685/716 (95%)	0.19	43 (6%) 20 28	17, 29, 60, 98	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	PRO	6.2
1	A	14	LEU	5.5
1	A	15	VAL	4.6
1	B	60	THR	4.6
1	B	57	GLY	4.5
1	B	59	LYS	4.4
1	B	243	LEU	4.4
1	B	192	GLU	3.6
1	B	147	ILE	3.6
1	B	55	ARG	3.6
1	B	78	ASP	3.5
1	A	17	ARG	3.3
1	A	18	GLY	3.3
1	B	19	SER	3.3
1	B	54	ASP	3.3
1	B	143[A]	CYS	3.3
1	B	196	ASN	3.2
1	B	152	ILE	3.0
1	B	186	SER	3.0
1	A	16	PRO	2.8
1	A	152	ILE	2.7
1	B	193	GLU	2.7
1	B	77	GLN	2.7
1	A	139	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	266	VAL	2.6
1	B	299	PHE	2.6
1	B	277	GLU	2.5
1	B	278	GLU	2.4
1	B	321	VAL	2.4
1	B	20	HIS	2.3
1	A	147	ILE	2.3
1	A	277	GLU	2.3
1	B	53	TYR	2.3
1	A	278	GLU	2.3
1	B	58	ILE	2.3
1	B	270	GLN	2.2
1	B	220	ASP	2.2
1	B	146	PHE	2.2
1	B	139	VAL	2.2
1	B	144	LEU	2.1
1	B	254	LEU	2.1
1	B	245	ARG	2.0
1	B	148	ASN	2.0

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 monosaccharides 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	GOL	B	401	6/6	0.84	0.30	50,54,59,60	0
2	GOL	A	401	6/6	0.89	0.20	42,48,55,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.