



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 AM UTC

PDB ID : 5VXD / pdb_00005vxd
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

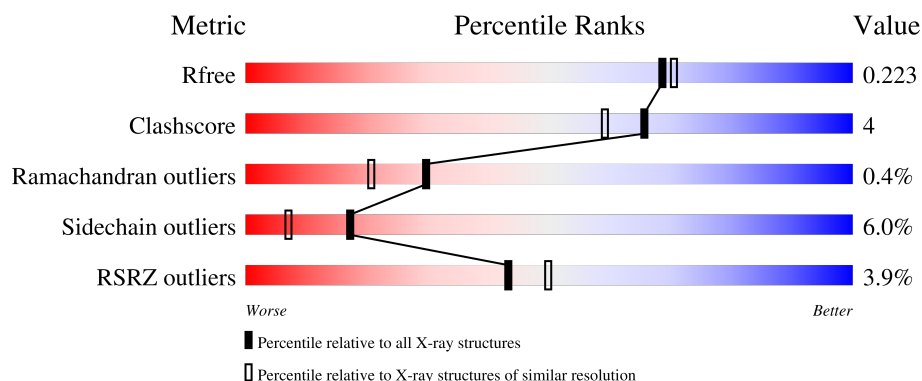
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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	2% 76% 19% • •
1	B	358	6% 73% 19% • • 5%

2 Entry composition

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
1	A	345	Total	C	N	O	S	0	3	0
			2641	1658	467	500	16			
1	B	340	Total	C	N	O	S	0	3	0
			2600	1631	459	494	16			

There are 42 discrepancies between the modelled and reference sequences:

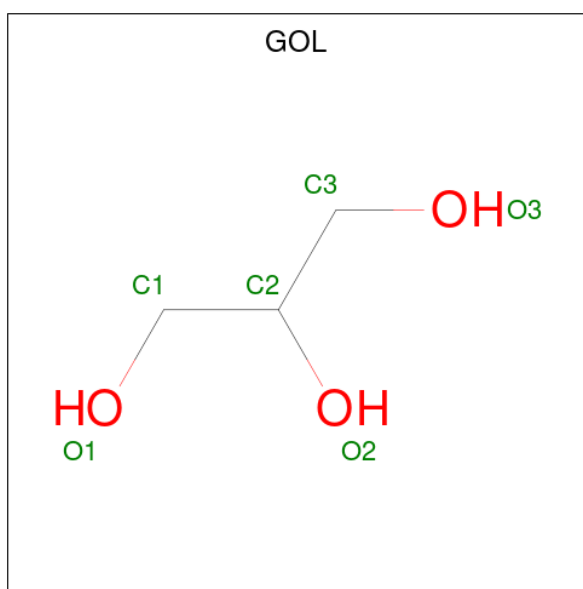
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8PDX2
A	2	GLY	-	expression tag	UNP Q8PDX2
A	3	SER	-	expression tag	UNP Q8PDX2
A	4	SER	-	expression tag	UNP Q8PDX2
A	5	HIS	-	expression tag	UNP Q8PDX2
A	6	HIS	-	expression tag	UNP Q8PDX2
A	7	HIS	-	expression tag	UNP Q8PDX2
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

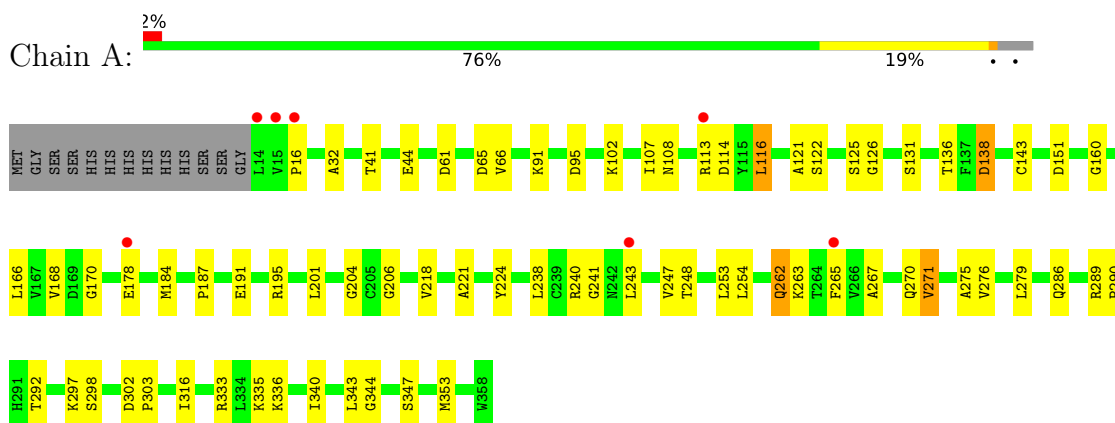
- Molecule 3 is water.

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

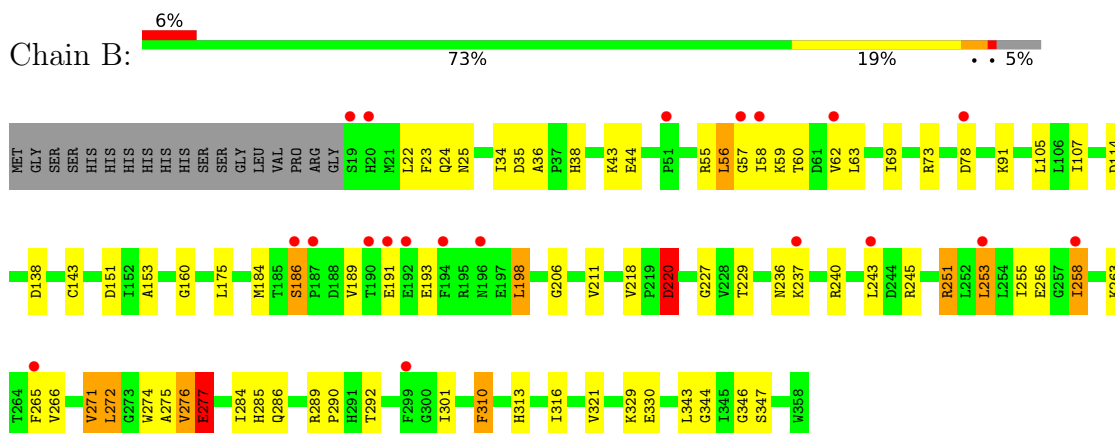
3 Residue-property plots [i](#)

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 50.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.97) 99.6 (50.00-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.97Å)	Xtriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
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

Xtriage'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	1.75	34/2681 (1.3%)	1.41	11/3630 (0.3%)
1	B	1.71	27/2639 (1.0%)	1.40	13/3573 (0.4%)
All	All	1.73	61/5320 (1.1%)	1.41	24/7203 (0.3%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ASP	CA-C	9.56	1.66	1.53
1	A	333	ARG	CZ-NH2	7.88	1.43	1.33
1	B	24	GLN	N-CA	7.19	1.55	1.45
1	A	138	ASP	CG-OD2	7.02	1.38	1.25
1	A	289	ARG	CA-C	6.99	1.60	1.52
1	A	204	GLY	N-CA	6.88	1.51	1.45
1	A	178	GLU	CG-CD	6.78	1.69	1.52
1	B	36	ALA	CA-C	6.77	1.61	1.53
1	A	126	GLY	N-CA	6.54	1.53	1.45
1	A	347	SER	CB-OG	-6.52	1.29	1.42
1	A	344	GLY	N-CA	6.47	1.52	1.45
1	B	175	LEU	C-O	6.39	1.31	1.24
1	B	34	ILE	C-O	6.35	1.30	1.24
1	B	114	ASP	C-O	-6.31	1.16	1.24
1	B	43	LYS	N-CA	6.29	1.54	1.46
1	B	151	ASP	C-O	-6.25	1.16	1.24
1	A	65	ASP	C-O	-6.22	1.16	1.24
1	A	168	VAL	C-O	6.22	1.30	1.24
1	B	344	GLY	N-CA	6.16	1.51	1.45
1	B	153	ALA	N-CA	-6.12	1.39	1.46
1	A	178	GLU	CB-CG	6.07	1.70	1.52
1	B	23	PHE	N-CA	5.87	1.53	1.46
1	A	160	GLY	C-O	-5.86	1.16	1.24
1	A	187	PRO	C-O	-5.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	LYS	C-O	-5.82	1.17	1.24
1	B	35	ASP	C-O	-5.78	1.17	1.24
1	B	321	VAL	CA-C	-5.75	1.46	1.52
1	A	206	GLY	N-CA	5.75	1.51	1.45
1	A	292	THR	C-O	-5.75	1.17	1.24
1	A	32	ALA	C-O	5.75	1.30	1.23
1	A	279	LEU	CA-C	-5.73	1.45	1.52
1	A	297	LYS	C-O	-5.69	1.17	1.24
1	A	95	ASP	CA-C	5.68	1.60	1.52
1	B	256	GLU	CA-C	5.67	1.60	1.52
1	A	114	ASP	CA-C	5.66	1.60	1.52
1	B	138	ASP	CG-OD2	5.65	1.36	1.25
1	B	236	ASN	CA-C	5.64	1.60	1.52
1	B	229	THR	CA-C	5.63	1.59	1.52
1	A	116	LEU	C-O	-5.59	1.17	1.24
1	B	220	ASP	CG-OD1	5.56	1.35	1.25
1	A	66	VAL	C-O	-5.55	1.18	1.24
1	A	61	ASP	C-O	5.53	1.30	1.24
1	A	290	PRO	C-O	-5.50	1.17	1.24
1	A	131	SER	CA-C	5.47	1.60	1.53
1	B	258	ILE	C-O	5.43	1.30	1.24
1	B	206	GLY	N-CA	5.41	1.50	1.45
1	A	298	SER	CA-C	-5.39	1.45	1.52
1	B	211	VAL	C-O	5.32	1.30	1.24
1	A	107	ILE	CA-CB	-5.31	1.47	1.54
1	A	91	LYS	CA-C	-5.30	1.45	1.52
1	A	122	SER	C-O	-5.27	1.17	1.24
1	A	340	ILE	C-O	5.22	1.29	1.24
1	B	160	GLY	C-O	-5.20	1.17	1.24
1	A	16	PRO	CA-C	5.17	1.58	1.52
1	B	310	PHE	CA-C	5.15	1.59	1.52
1	A	170	GLY	C-O	-5.10	1.17	1.23
1	B	301	ILE	C-O	-5.09	1.17	1.24
1	B	285	HIS	N-CA	-5.06	1.39	1.46
1	B	44	GLU	N-CA	5.05	1.52	1.46
1	A	247	VAL	CA-CB	-5.01	1.48	1.54
1	A	333	ARG	NE-CZ	5.01	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLU	CB-CG-CD	9.46	128.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	GLY	CA-C-O	-7.35	115.20	120.94
1	A	286	GLN	N-CA-C	6.80	120.02	109.07
1	B	265	PHE	N-CA-C	6.76	119.22	111.11
1	B	78	ASP	N-CA-C	6.40	120.35	111.90
1	A	347	SER	CB-CA-C	6.03	119.74	109.72
1	A	178	GLU	N-CA-CB	5.99	119.02	110.16
1	A	298	SER	CB-CA-C	-5.97	100.88	110.79
1	B	266	VAL	CB-CA-C	-5.92	104.15	112.14
1	B	276	VAL	N-CA-C	-5.90	101.14	109.63
1	B	253	LEU	CA-CB-CG	5.85	136.78	116.30
1	A	121	ALA	N-CA-C	5.58	118.08	111.33
1	B	274	TRP	N-CA-C	5.57	118.39	110.10
1	A	275	ALA	N-CA-C	-5.46	100.88	109.50
1	B	58	ILE	N-CA-C	-5.43	102.57	109.58
1	A	238	LEU	N-CA-C	5.36	117.12	111.28
1	B	22	LEU	N-CA-C	-5.27	103.73	110.53
1	B	275	ALA	CA-C-N	5.25	127.53	120.50
1	B	275	ALA	C-N-CA	5.25	127.53	120.50
1	A	241	GLY	O-C-N	5.11	127.37	123.23
1	B	63	LEU	CA-C-N	5.06	125.45	119.94
1	B	63	LEU	C-N-CA	5.06	125.45	119.94
1	A	221	ALA	CA-C-N	5.05	124.97	119.76
1	A	221	ALA	C-N-CA	5.05	124.97	119.76

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	1	0
3	B	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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: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
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:254:LEU:C	1:A:254:LEU:HD23	2.38	0.48
1:A:262[A]:GLN:HG2	1:A:263:LYS:N	2.29	0.48
1:B:184:MET:HE1	1:B:198:LEU:HA	1.97	0.47
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:151:ASP:OD1	1:A:224:TYR:OH	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:CD2	1:A:353:MET:HE1	2.55	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%)	14	6
All	All	687/716 (96%)	661 (96%)	23 (3%)	3 (0%)	30	21

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%)	270 (96%)	11 (4%)	28	18
1	B	277/289 (96%)	253 (91%)	24 (9%)	9	2
All	All	558/578 (96%)	523 (94%)	35 (6%)	17	6

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

Mol	Chain	Res	Type
1	A	102	LYS
1	A	143[A]	CYS
1	A	143[B]	CYS
1	A	166	LEU
1	A	243	LEU
1	A	262[A]	GLN
1	A	262[B]	GLN
1	A	271	VAL
1	A	276	VAL
1	A	335	LYS
1	A	336	LYS
1	B	56	LEU
1	B	59	LYS
1	B	60	THR
1	B	62	VAL
1	B	91	LYS
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	258	ILE
1	B	263	LYS
1	B	271	VAL
1	B	272	LEU
1	B	277	GLU
1	B	286	GLN
1	B	330	GLU
1	B	343	LEU

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Mol	Chain	Res	Type
1	B	347	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	270	GLN
1	B	97	ASN
1	B	270	GLN
1	B	285	HIS
1	B	350	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.29	0	5,5,5	1.34	1 (20%)
2	GOL	B	401	-	5,5,5	0.43	0	5,5,5	0.69	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	2.20	118.28	109.18

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 [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	345/358 (96%)	-0.16	7 (2%) 65 72	13, 28, 46, 74	3 (0%)
1	B	340/358 (94%)	0.18	20 (5%) 28 32	10, 31, 71, 98	3 (0%)
All	All	685/716 (95%)	0.01	27 (3%) 43 50	10, 29, 60, 98	6 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	6.3
1	B	187	PRO	5.2
1	B	243	LEU	4.1
1	B	299	PHE	3.0
1	B	19	SER	3.0
1	B	20	HIS	2.9
1	B	196	ASN	2.8
1	A	15	VAL	2.7
1	B	194	PHE	2.6
1	B	58	ILE	2.6
1	B	51	PRO	2.4
1	B	192	GLU	2.4
1	B	190	THR	2.4
1	B	253	LEU	2.4
1	B	265	PHE	2.4
1	A	113	ARG	2.3
1	B	258	ILE	2.3
1	A	265	PHE	2.2
1	B	78	ASP	2.2
1	A	243	LEU	2.2
1	A	16	PRO	2.2
1	B	57	GLY	2.2
1	B	186	SER	2.2
1	B	62	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	237	LYS	2.1
1	B	191	GLU	2.1
1	A	178	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	401	6/6	0.87	0.16	50,54,59,60	0
2	GOL	A	401	6/6	0.90	0.13	42,48,55,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.