



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:03 PM UTC

PDB ID : 5VXH / pdb_00005vxh
Title : Crystal structure of Xanthomonas campestris OleA E117D
Authors : Jensen, M.R.; Wilmot, C.M.
Deposited on : 2017-05-23
Resolution : 1.84 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

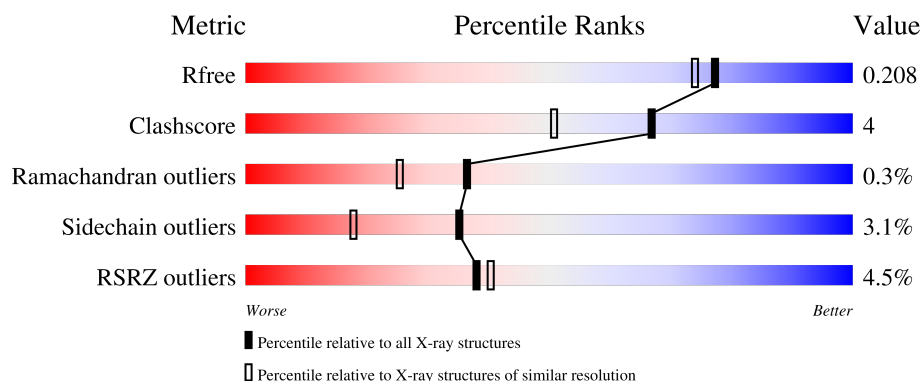
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	8% 83% 11% • •
1	B	358	8% 73% 15% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5419 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	5	0
			2657	1669	467	506	15			
1	B	326	Total	C	N	O	S	0	4	0
			2507	1580	437	476	14			

There are 42 discrepancies between the modelled and reference sequences:

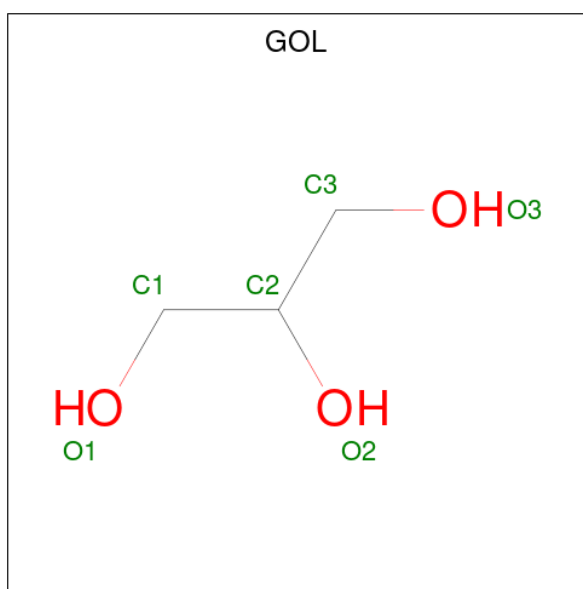
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8PDX2
A	2	GLY	-	expression tag	UNP Q8PDX2
A	3	SER	-	expression tag	UNP Q8PDX2
A	4	SER	-	expression tag	UNP Q8PDX2
A	5	HIS	-	expression tag	UNP Q8PDX2
A	6	HIS	-	expression tag	UNP Q8PDX2
A	7	HIS	-	expression tag	UNP Q8PDX2
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	ASP	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	ASP	GLU	engineered mutation	UNP Q8PDX2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



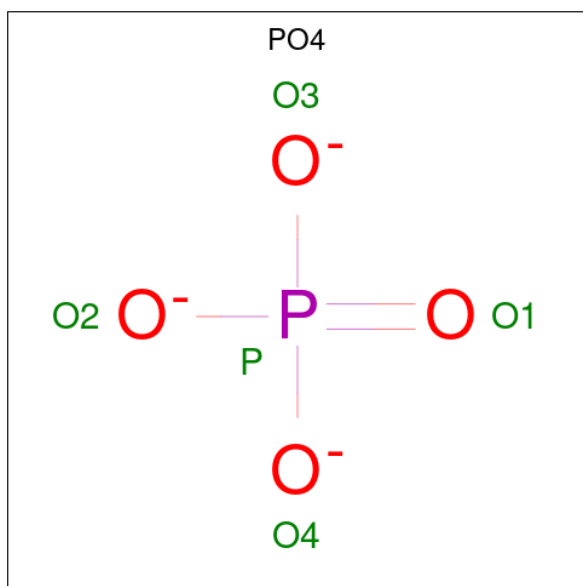
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

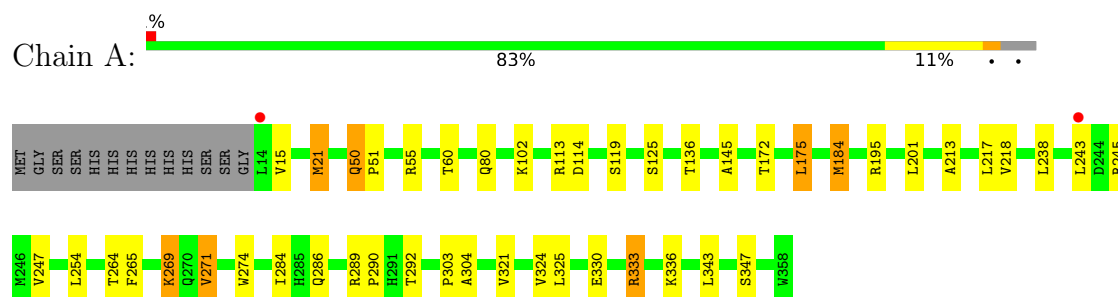
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	88	Total	O	0	0
			88	88		

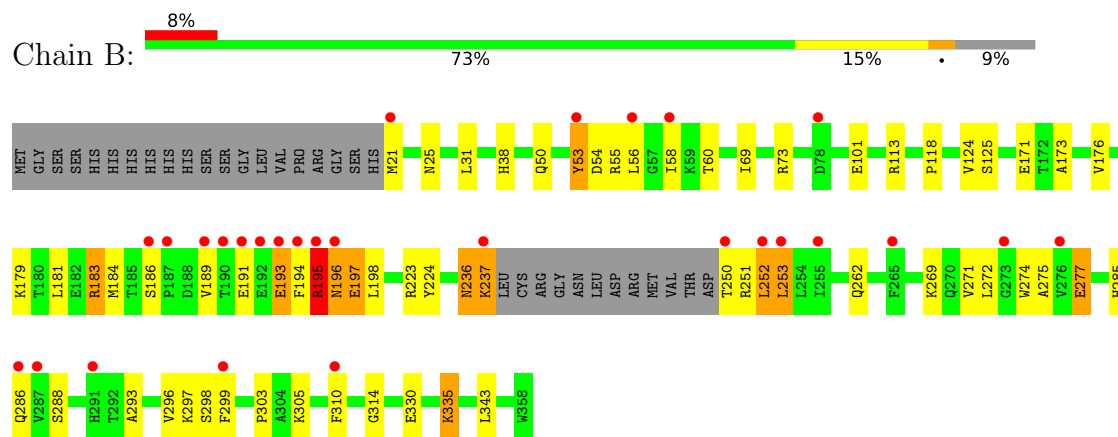
3 Residue-property plots

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	81.88Å 85.41Å 102.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.84 50.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.84) 100.0 (50.00-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.158 , 0.198 0.171 , 0.208	Depositor DCC
R_{free} test set	3170 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5419	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, PO4

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	1.67	21/2700 (0.8%)	1.37	12/3657 (0.3%)
1	B	1.70	23/2545 (0.9%)	1.48	23/3445 (0.7%)
All	All	1.69	44/5245 (0.8%)	1.43	35/7102 (0.5%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	TYR	N-CA	7.26	1.55	1.46
1	B	285	HIS	C-O	-7.24	1.15	1.23
1	B	124	VAL	CA-C	7.12	1.61	1.52
1	A	264	THR	CA-C	6.73	1.61	1.52
1	A	15	VAL	N-CA	6.72	1.52	1.46
1	B	101	GLU	CD-OE1	6.69	1.38	1.25
1	B	171	GLU	N-CA	-6.62	1.38	1.46
1	B	53	TYR	CA-C	6.57	1.61	1.52
1	B	296	VAL	CA-C	6.54	1.60	1.52
1	A	304	ALA	C-O	-6.41	1.15	1.24
1	A	265	PHE	CA-C	-6.30	1.44	1.52
1	A	347	SER	C-O	6.24	1.31	1.23
1	B	25	ASN	CG-OD1	6.23	1.35	1.23
1	B	251	ARG	CA-C	6.17	1.61	1.52
1	A	114	ASP	CA-C	6.11	1.60	1.52
1	B	288	SER	CA-C	-6.03	1.45	1.52
1	B	343	LEU	CA-C	-5.98	1.45	1.52
1	A	195	ARG	C-O	-5.84	1.17	1.24
1	A	247	VAL	C-O	5.80	1.30	1.24
1	A	286	GLN	N-CA	5.79	1.53	1.46
1	B	50	GLN	CA-C	5.77	1.59	1.52
1	B	181	LEU	CA-C	5.75	1.60	1.52
1	A	125	SER	CA-CB	5.72	1.62	1.53
1	B	303	PRO	N-CA	5.50	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	LYS	CA-C	-5.48	1.45	1.52
1	A	50	GLN	CD-OE1	5.48	1.33	1.23
1	B	25	ASN	N-CA	5.46	1.54	1.46
1	A	55	ARG	N-CA	-5.40	1.39	1.46
1	B	183	ARG	CA-C	-5.39	1.46	1.52
1	B	286	GLN	C-O	5.37	1.30	1.24
1	B	286	GLN	CA-CB	-5.36	1.45	1.53
1	B	193	GLU	CA-CB	5.34	1.62	1.53
1	A	321	VAL	CA-CB	5.33	1.57	1.54
1	A	119	SER	CA-C	5.27	1.59	1.52
1	A	136	THR	C-O	-5.27	1.17	1.23
1	B	335	LYS	C-O	5.27	1.30	1.23
1	A	175	LEU	N-CA	-5.26	1.40	1.46
1	A	213	ALA	N-CA	5.13	1.52	1.45
1	B	293	ALA	N-CA	5.11	1.52	1.46
1	A	324	VAL	C-O	5.08	1.30	1.24
1	A	271	VAL	N-CA	-5.06	1.39	1.46
1	B	31	LEU	CB-CG	-5.03	1.43	1.53
1	A	303	PRO	N-CA	5.02	1.54	1.47
1	A	217	LEU	N-CA	-5.01	1.39	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	VAL	N-CA-C	7.86	119.91	111.58
1	B	191	GLU	N-CA-C	7.62	120.47	111.71
1	B	286	GLN	CA-C-N	6.72	129.18	122.66
1	B	286	GLN	C-N-CA	6.72	129.18	122.66
1	B	196	ASN	N-CA-C	-6.62	100.85	110.64
1	B	252	LEU	CA-C-O	-6.46	113.99	120.90
1	A	271	VAL	CG1-CB-CG2	6.46	125.00	110.80
1	B	272	LEU	N-CA-C	6.31	121.12	113.17
1	B	125	SER	CA-CB-OG	-6.28	98.55	111.10
1	B	236	ASN	N-CA-C	-6.24	104.58	111.82
1	B	253	LEU	CB-CA-C	-6.20	100.89	110.81
1	A	184	MET	CG-SD-CE	-6.20	87.27	100.90
1	B	298	SER	CB-CA-C	-6.07	100.71	110.79
1	A	15	VAL	N-CA-C	5.90	114.38	107.77
1	B	195	ARG	CA-C-O	-5.87	112.12	120.51
1	B	252	LEU	N-CA-CB	5.82	118.62	109.94
1	B	274	TRP	N-CA-C	5.66	118.56	110.24
1	B	330	GLU	CA-CB-CG	-5.59	102.92	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ARG	CG-CD-NE	-5.52	99.87	112.00
1	B	286	GLN	O-C-N	5.43	130.29	123.12
1	A	113	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	113	ARG	CB-CG-CD	5.33	123.55	111.30
1	A	136	THR	OG1-CB-CG2	-5.28	98.73	109.30
1	B	305	LYS	CD-CE-NZ	-5.21	95.22	111.90
1	A	254	LEU	N-CA-C	5.15	116.59	110.97
1	A	238	LEU	N-CA-C	5.13	117.61	111.71
1	B	21	MET	CB-CA-C	5.13	119.85	110.10
1	A	145	ALA	N-CA-C	5.08	117.55	111.71
1	B	101	GLU	CG-CD-OE2	-5.08	106.71	118.40
1	B	196	ASN	CA-C-N	5.08	131.24	121.54
1	B	196	ASN	C-N-CA	5.08	131.24	121.54
1	B	183	ARG	CB-CA-C	-5.04	102.91	110.92
1	A	60	THR	OG1-CB-CG2	-5.02	99.26	109.30
1	A	325	LEU	CA-C-N	5.00	126.94	120.44
1	A	325	LEU	C-N-CA	5.00	126.94	120.44

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	2657	0	2693	19	0
1	B	2507	0	2536	20	0
2	A	18	0	24	1	0
2	B	6	0	8	0	0
3	A	5	0	0	0	0
4	A	138	0	0	2	0
4	B	88	0	0	0	0
All	All	5419	0	5261	39	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 (39) 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:175:LEU:HD23	1:A:243:LEU:HG	1.62	0.82
1:B:262:GLN:HG2	1:B:299:PHE:HE1	1.46	0.79
1:A:284[B]:ILE:O	1:A:284[B]:ILE:HG13	1.87	0.74
1:A:333:ARG:NH1	4:A:501:HOH:O	2.19	0.73
1:B:194:PHE:O	1:B:195:ARG:O	2.12	0.67
1:A:284[B]:ILE:O	1:A:284[B]:ILE:CG1	2.42	0.66
1:B:262:GLN:HG2	1:B:299:PHE:CE1	2.30	0.66
1:A:184:MET:HE1	1:A:201:LEU:HD11	1.79	0.63
1:B:54:ASP:C	1:B:55:ARG:O	2.40	0.61
1:B:277:GLU:CD	1:B:277:GLU:H	2.10	0.60
1:B:184:MET:HE3	1:B:197:GLU:HG2	1.87	0.57
1:A:284[B]:ILE:HD11	1:A:292:THR:HG23	1.87	0.57
1:B:69:ILE:HB	1:B:310[A]:PHE:CE2	2.39	0.57
1:B:262:GLN:CG	1:B:299:PHE:CE1	2.91	0.54
1:B:183:ARG:HG2	1:B:193:GLU:OE1	2.09	0.53
1:B:69:ILE:HD12	1:B:314:GLY:HA2	1.92	0.52
1:A:184:MET:HE1	1:A:201:LEU:CD1	2.39	0.51
1:B:195:ARG:O	1:B:196:ASN:C	2.54	0.50
1:B:186:SER:HB2	1:B:189:VAL:HG23	1.94	0.49
1:A:184:MET:CE	1:A:201:LEU:HD11	2.41	0.49
1:B:252:LEU:HD23	1:B:253:LEU:H	1.78	0.48
1:A:269:LYS:HE3	1:A:274:TRP:O	2.15	0.47
1:B:173:ALA:O	1:B:176:VAL:HG12	2.15	0.46
1:A:269:LYS:HG2	1:A:274:TRP:O	2.15	0.46
1:A:172:THR:HB	4:A:504:HOH:O	2.16	0.45
1:A:102:LYS:HA	1:A:102:LYS:HD3	1.66	0.45
1:B:184:MET:HE1	1:B:198:LEU:HA	1.99	0.45
1:A:218:VAL:O	1:A:218:VAL:HG23	2.17	0.44
1:B:55:ARG:NH1	1:B:56:LEU:HD21	2.32	0.43
1:A:284[B]:ILE:HG22	1:A:343:LEU:HD13	2.00	0.43
1:B:275:ALA:HB1	1:B:277:GLU:OE2	2.20	0.41
1:A:289:ARG:HB3	1:A:290:PRO:HD3	2.03	0.41
1:A:184:MET:HE3	1:A:184:MET:HB3	1.82	0.41
1:A:245:ARG:HH11	1:A:245:ARG:HD3	1.73	0.41
1:B:53:TYR:HD1	1:B:58:ILE:HB	1.86	0.41
1:B:236:ASN:HD21	1:B:237:LYS:HE2	1.86	0.41
1:A:50:GLN:HB3	1:A:51:PRO:HD3	2.02	0.41
1:B:38:HIS:O	1:B:73:ARG:HA	2.22	0.40
1:A:21:MET:HG3	2:A:402:GOL:H32	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/358 (97%)	338 (97%)	10 (3%)	0	100	100
1	B	326/358 (91%)	311 (95%)	13 (4%)	2 (1%)	21	9
All	All	674/716 (94%)	649 (96%)	23 (3%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	ARG
1	B	197	GLU

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	284/290 (98%)	277 (98%)	7 (2%)	42	24
1	B	266/290 (92%)	256 (96%)	10 (4%)	29	12
All	All	550/580 (95%)	533 (97%)	17 (3%)	35	18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	80	GLN
1	A	269	LYS
1	A	271	VAL

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Mol	Chain	Res	Type
1	A	330	GLU
1	A	333	ARG
1	A	336	LYS
1	B	60	THR
1	B	118	PRO
1	B	195	ARG
1	B	237	LYS
1	B	250	THR
1	B	269	LYS
1	B	271	VAL
1	B	277	GLU
1	B	297	LYS
1	B	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	GLN
1	B	87	GLN
1	B	236	ASN
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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	404	-	4,4,4	0.84	0	6,6,6	0.86	0
2	GOL	A	402	-	5,5,5	0.69	0	5,5,5	0.86	0
2	GOL	B	401	-	5,5,5	0.99	0	5,5,5	1.03	0
2	GOL	A	401	-	5,5,5	0.34	0	5,5,5	1.44	0
2	GOL	A	403	-	5,5,5	0.37	0	5,5,5	0.77	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	403	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	1	0

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%)	-0.31	2 (0%) 85 90	11, 23, 39, 58	5 (1%)
1	B	326/358 (91%)	0.10	28 (8%) 16 17	10, 26, 59, 79	4 (1%)
All	All	671/716 (93%)	-0.11	30 (4%) 38 40	10, 24, 53, 79	9 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	6.3
1	B	250	THR	4.2
1	B	189	VAL	4.0
1	B	253	LEU	4.0
1	B	187	PRO	4.0
1	B	252	LEU	3.9
1	B	192	GLU	3.5
1	B	196	ASN	3.5
1	B	56	LEU	3.5
1	B	58	ILE	3.2
1	B	191	GLU	3.1
1	A	243	LEU	3.0
1	B	53	TYR	2.9
1	B	193	GLU	2.8
1	B	186	SER	2.8
1	B	310[A]	PHE	2.8
1	B	195	ARG	2.8
1	B	237	LYS	2.8
1	B	273	GLY	2.6
1	B	291	HIS	2.5
1	B	255	ILE	2.4
1	B	265	PHE	2.4
1	B	21	MET	2.4
1	B	299	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	190	THR	2.3
1	B	194	PHE	2.2
1	B	287	VAL	2.1
1	B	286	GLN	2.1
1	B	276	VAL	2.1
1	B	78	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	PO4	A	404	5/5	0.68	0.17	61,73,79,85	0
2	GOL	A	401	6/6	0.90	0.10	34,38,39,39	0
2	GOL	A	403	6/6	0.91	0.10	33,39,44,47	0
2	GOL	B	401	6/6	0.93	0.09	28,30,31,34	0
2	GOL	A	402	6/6	0.94	0.09	25,33,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.