



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:55 PM UTC

PDB ID : 5VXF / pdb_00005vxf
Title : Crystal structure of Xanthomonas campestris OleA E117Q
Authors : Jensen, M.R.; Wilmot, C.M.
Deposited on : 2017-05-23
Resolution : 1.75 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

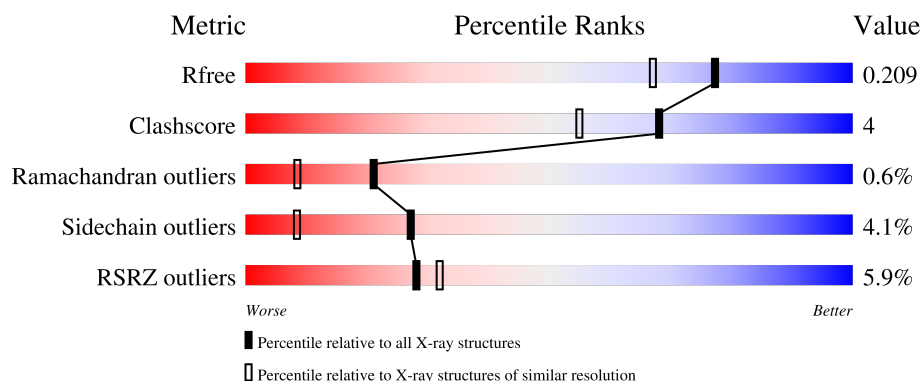
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	% 80% 15% • •
1	B	358	10% 72% 17% • • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5475 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	9	0
			2697	1697	473	510	17			
1	B	328	Total	C	N	O	S	0	6	0
			2539	1597	445	483	14			

There are 42 discrepancies between the modelled and reference sequences:

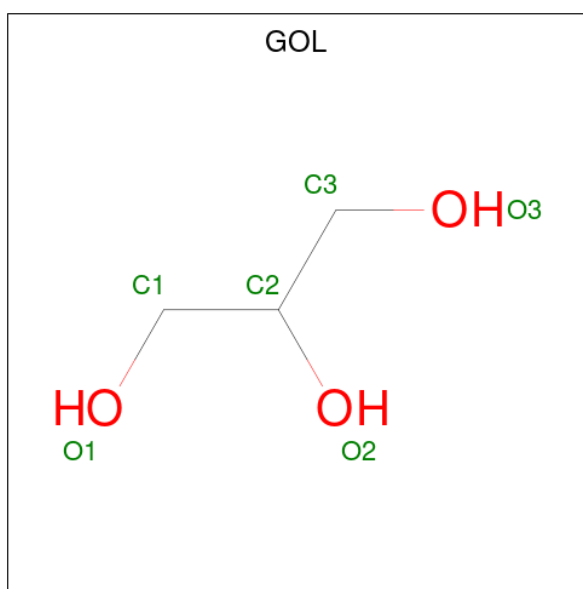
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8PDX2
A	2	GLY	-	expression tag	UNP Q8PDX2
A	3	SER	-	expression tag	UNP Q8PDX2
A	4	SER	-	expression tag	UNP Q8PDX2
A	5	HIS	-	expression tag	UNP Q8PDX2
A	6	HIS	-	expression tag	UNP Q8PDX2
A	7	HIS	-	expression tag	UNP Q8PDX2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

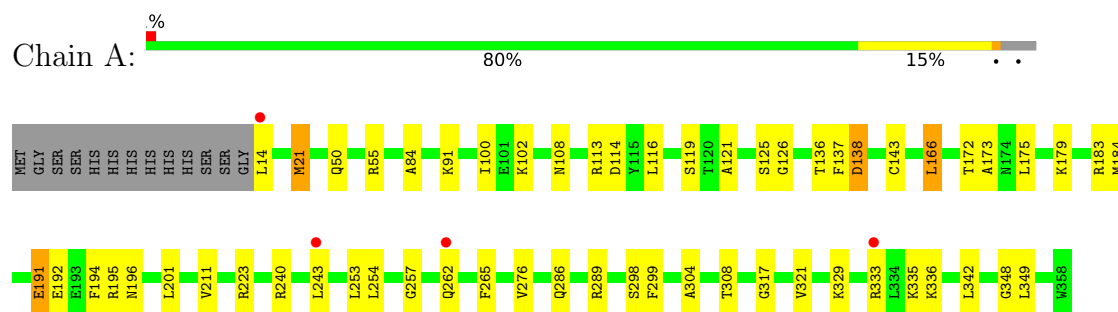
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	1
			132	132		
3	B	83	Total	O	0	0
			83	83		

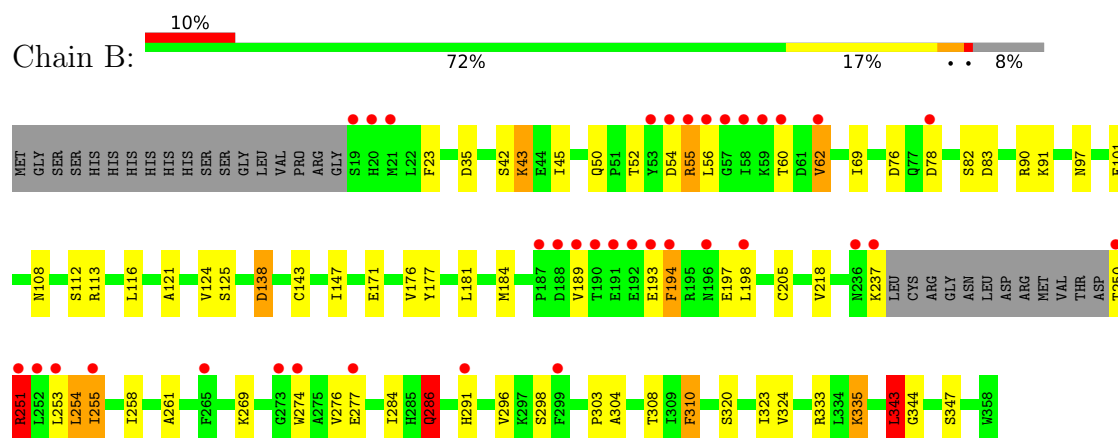
3 Residue-property plots [i](#)

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	82.24Å 85.86Å 102.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.75) 99.6 (50.00-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.161 , 0.197 0.173 , 0.209	Depositor DCC
R_{free} test set	3718 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.6	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	0.97	EDS
Total number of atoms	5475	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	1.79	30/2739 (1.1%)	1.42	10/3708 (0.3%)
1	B	1.80	36/2577 (1.4%)	1.48	16/3488 (0.5%)
All	All	1.80	66/5316 (1.2%)	1.45	26/7196 (0.4%)

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	1
1	B	0	2
All	All	0	3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ARG	CZ-NH1	9.66	1.46	1.32
1	B	251	ARG	CA-C	9.50	1.61	1.52
1	B	251	ARG	N-CA	8.40	1.56	1.46
1	B	138	ASP	CG-OD2	7.57	1.39	1.25
1	B	112	SER	C-O	-7.31	1.15	1.23
1	A	125	SER	CA-CB	7.12	1.64	1.53
1	A	333	ARG	NE-CZ	7.05	1.40	1.33
1	B	343	LEU	CA-C	-6.96	1.44	1.52
1	B	113	ARG	N-CA	6.92	1.54	1.45
1	A	166	LEU	N-CA	-6.92	1.37	1.46
1	A	191	GLU	N-CA	-6.91	1.37	1.46
1	A	138	ASP	CG-OD2	6.80	1.38	1.25
1	B	344	GLY	N-CA	6.80	1.52	1.45
1	A	223	ARG	CD-NE	6.78	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	LYS	N-CA	-6.71	1.37	1.46
1	A	240	ARG	CD-NE	-6.65	1.36	1.46
1	B	335	LYS	C-O	6.39	1.32	1.23
1	B	78	ASP	CA-C	6.33	1.61	1.52
1	B	101	GLU	CD-OE1	6.30	1.37	1.25
1	B	261	ALA	N-CA	6.22	1.53	1.46
1	A	211	VAL	CA-CB	-6.18	1.47	1.54
1	A	333	ARG	CD-NE	6.09	1.54	1.46
1	B	91	LYS	C-O	-6.09	1.16	1.24
1	A	84	ALA	N-CA	6.02	1.53	1.46
1	A	257	GLY	CA-C	-6.01	1.45	1.52
1	A	138	ASP	CA-C	5.99	1.60	1.52
1	A	304	ALA	C-O	-5.96	1.16	1.24
1	B	181	LEU	CA-C	5.94	1.60	1.52
1	B	296	VAL	N-CA	-5.84	1.39	1.46
1	B	310	PHE	CB-CG	-5.78	1.37	1.50
1	A	100	ILE	C-O	5.76	1.31	1.24
1	B	171	GLU	N-CA	-5.67	1.39	1.46
1	B	23	PHE	N-CA	5.63	1.53	1.46
1	B	320	SER	N-CA	5.57	1.53	1.46
1	B	324	VAL	N-CA	5.55	1.53	1.46
1	B	143	CYS	N-CA	-5.54	1.38	1.46
1	B	124	VAL	CA-CB	-5.46	1.48	1.54
1	B	83	ASP	N-CA	5.44	1.53	1.46
1	A	298	SER	CA-C	-5.43	1.45	1.52
1	A	175	LEU	N-CA	-5.43	1.39	1.46
1	B	205	CYS	C-O	5.43	1.30	1.23
1	A	173	ALA	N-CA	5.42	1.52	1.46
1	A	183	ARG	NE-CZ	5.42	1.39	1.33
1	B	276	VAL	CA-C	-5.41	1.45	1.52
1	A	55	ARG	CZ-NH2	-5.40	1.26	1.33
1	B	323	ILE	CA-C	5.38	1.59	1.52
1	B	255	ILE	CA-CB	5.37	1.61	1.54
1	A	329	LYS	C-O	5.36	1.30	1.24
1	B	304	ALA	CA-CB	-5.34	1.44	1.53
1	B	101	GLU	C-O	-5.33	1.17	1.24
1	B	45	ILE	CA-CB	-5.32	1.47	1.54
1	B	35	ASP	N-CA	5.32	1.52	1.46
1	B	218	VAL	N-CA	5.25	1.53	1.46
1	A	196	ASN	CA-CB	5.22	1.61	1.53
1	A	50	GLN	CD-OE1	5.22	1.33	1.23
1	A	114	ASP	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	VAL	CA-CB	-5.18	1.51	1.54
1	B	43	LYS	N-CA	5.16	1.52	1.46
1	A	192	GLU	CA-C	5.16	1.59	1.52
1	B	177	TYR	CA-CB	5.16	1.61	1.53
1	A	137	PHE	CA-C	-5.10	1.46	1.52
1	B	343	LEU	CA-CB	-5.10	1.44	1.53
1	A	136	THR	N-CA	5.09	1.52	1.46
1	B	303	PRO	N-CA	5.07	1.54	1.47
1	A	126	GLY	N-CA	5.02	1.52	1.45
1	B	121	ALA	N-CA	-5.00	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ARG	CA-C-O	8.61	129.89	119.81
1	A	333	ARG	CB-CG-CD	8.09	129.91	111.30
1	A	333	ARG	NE-CZ-NH1	7.14	128.64	121.50
1	B	251	ARG	N-CA-C	6.61	121.18	112.72
1	B	125	SER	CA-CB-OG	-6.16	98.78	111.10
1	B	62	VAL	N-CA-C	6.08	116.82	110.62
1	B	82	SER	N-CA-C	5.98	117.80	111.28
1	A	289	ARG	CA-C-N	-5.87	112.96	119.19
1	A	289	ARG	C-N-CA	-5.87	112.96	119.19
1	A	172	THR	OG1-CB-CG2	-5.87	97.56	109.30
1	A	333	ARG	N-CA-CB	5.87	120.13	110.39
1	B	143	CYS	N-CA-C	5.76	120.17	113.20
1	A	138	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	333	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	B	90	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	B	147	ILE	N-CA-C	-5.51	105.16	110.72
1	B	274	TRP	N-CA-C	5.41	118.08	109.96
1	A	191	GLU	CB-CG-CD	-5.35	103.50	112.60
1	B	101	GLU	CG-CD-OE1	5.32	130.64	118.40
1	A	342	LEU	N-CA-C	-5.19	100.07	108.52
1	B	343	LEU	N-CA-C	5.17	116.93	109.07
1	B	50	GLN	O-C-N	5.04	124.97	120.48
1	B	286[A]	GLN	CA-C-O	-5.03	115.12	120.40
1	B	286[B]	GLN	CA-C-O	-5.03	115.12	120.40
1	B	50	GLN	N-CA-CB	5.01	117.77	110.30
1	A	121	ALA	N-CA-C	5.00	117.39	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	SER	Mainchain
1	B	250	THR	Peptide
1	B	251	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2697	0	2724	20	0
1	B	2539	0	2566	19	0
2	A	12	0	16	1	0
2	B	12	0	16	3	0
3	A	132	0	0	1	0
3	B	83	0	0	0	0
All	All	5475	0	5322	38	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 (38) 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:253[B]:LEU:HD13	1:A:253[B]:LEU:O	1.67	0.93
1:A:253[B]:LEU:HD13	1:A:253[B]:LEU:C	2.01	0.84
1:A:253[B]:LEU:C	1:A:253[B]:LEU:CD1	2.62	0.73
1:A:184[A]:MET:HE1	1:A:201:LEU:HD11	1.79	0.65
1:B:62:VAL:HG11	1:B:198:LEU:HD13	1.80	0.62
1:B:184:MET:HE3	1:B:197:GLU:CB	2.30	0.61
1:B:284[B]:ILE:HG22	1:B:343:LEU:HG	1.83	0.59
1:B:286[B]:GLN:HE22	1:B:308:THR:HG22	1.66	0.59
1:B:184:MET:HE3	1:B:197:GLU:HB3	1.85	0.58
1:A:113:ARG:CZ	1:A:116:LEU:HD23	2.35	0.57
1:A:265[B]:PHE:CZ	1:A:276:VAL:HG23	2.40	0.57
1:A:254:LEU:C	1:A:254:LEU:HD23	2.30	0.56
1:A:143[B]:CYS:SG	1:A:317:GLY:HA2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HG11	1:B:198:LEU:CD1	2.38	0.53
1:B:284[B]:ILE:CG1	1:B:286[B]:GLN:HE21	2.22	0.53
1:A:286:GLN:OE1	1:A:308[B]:THR:HB	2.11	0.50
1:B:286[B]:GLN:NE2	1:B:308:THR:HG22	2.27	0.50
1:B:52:THR:HG21	1:B:194:PHE:CE1	2.47	0.49
1:B:43:LYS:N	2:B:402:GOL:H31	2.27	0.49
1:B:55:ARG:NH2	1:B:189:VAL:O	2.43	0.48
1:B:54:ASP:C	1:B:56:LEU:H	2.23	0.47
1:B:284[B]:ILE:HG13	1:B:286[B]:GLN:HE21	1.80	0.46
1:A:243:LEU:HD23	1:B:116:LEU:HD11	1.96	0.46
1:A:108:ASN:HB3	1:A:138:ASP:OD1	2.17	0.45
1:A:191:GLU:HG2	1:A:195:ARG:CZ	2.46	0.45
1:B:42:SER:HB2	2:B:402:GOL:H31	1.99	0.44
1:A:262:GLN:HG2	1:A:299[A]:PHE:HE1	1.82	0.44
1:A:143[A]:CYS:HB3	3:A:623:HOH:O	2.17	0.44
1:A:348:GLY:N	1:A:349:LEU:HA	2.33	0.44
1:A:184[A]:MET:HB2	1:A:184[A]:MET:HE2	1.38	0.43
1:B:254:LEU:HB2	1:B:291:HIS:NE2	2.33	0.43
1:B:42:SER:HB2	2:B:402:GOL:C3	2.49	0.42
1:A:184[B]:MET:HE2	1:A:194:PHE:CE1	2.55	0.41
1:A:21:MET:HA	2:A:401:GOL:H32	2.01	0.41
1:B:69:ILE:HB	1:B:310:PHE:CE2	2.55	0.41
1:A:253[B]:LEU:HD22	1:A:349:LEU:HD21	2.02	0.40
1:B:108:ASN:HB3	1:B:138:ASP:OD1	2.21	0.40
1:A:91:LYS:HE2	1:A:91:LYS:HB3	1.96	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	352/358 (98%)	343 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	330/358 (92%)	312 (94%)	14 (4%)	4 (1%)	10	2
All	All	682/716 (95%)	655 (96%)	23 (3%)	4 (1%)	21	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ARG
1	B	76	ASP
1	B	193	GLU
1	B	194	PHE

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	288/290 (99%)	282 (98%)	6 (2%)	47	27
1	B	270/290 (93%)	253 (94%)	17 (6%)	16	3
All	All	558/580 (96%)	535 (96%)	23 (4%)	27	8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	21	MET
1	A	102	LYS
1	A	166	LEU
1	A	335	LYS
1	A	336	LYS
1	B	60	THR
1	B	97	ASN
1	B	176	VAL
1	B	237	LYS
1	B	251	ARG
1	B	253	LEU

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Mol	Chain	Res	Type
1	B	254	LEU
1	B	255	ILE
1	B	258	ILE
1	B	269	LYS
1	B	277	GLU
1	B	286[A]	GLN
1	B	286[B]	GLN
1	B	298	SER
1	B	335	LYS
1	B	343	LEU
1	B	347	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	108	ASN
1	B	350	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	B	402	-	5,5,5	0.81	0	5,5,5	2.33	2 (40%)
2	GOL	A	402	-	5,5,5	0.11	0	5,5,5	1.55	1 (20%)
2	GOL	A	401	-	5,5,5	0.66	0	5,5,5	1.38	1 (20%)
2	GOL	B	401	-	5,5,5	0.37	0	5,5,5	1.42	1 (20%)

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	B	402	-	-	3/4/4/4	-
2	GOL	A	402	-	-	3/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	GOL	O2-C2-C3	-3.88	93.12	109.18
2	B	401	GOL	O1-C1-C2	-2.86	97.49	110.38
2	B	402	GOL	O3-C3-C2	2.78	122.91	110.38
2	A	402	GOL	O2-C2-C3	2.49	119.50	109.18
2	A	401	GOL	O1-C1-C2	-2.41	99.53	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	B	402	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	B	401	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	401	GOL	O2-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GOL	3	0
2	A	401	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%)	-0.09	4 (1%) 76 82	12, 26, 42, 58	9 (2%)
1	B	328/358 (91%)	0.39	36 (10%) 10 11	11, 29, 67, 98	6 (1%)
All	All	673/716 (93%)	0.14	40 (5%) 28 32	11, 27, 57, 98	15 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	7.3
1	B	253	LEU	5.2
1	B	189	VAL	4.5
1	B	20	HIS	4.4
1	B	58	ILE	4.3
1	B	187	PRO	4.3
1	B	250	THR	3.9
1	B	57	GLY	3.6
1	B	237	LYS	3.6
1	B	194	PHE	3.4
1	B	252	LEU	3.4
1	B	255	ILE	3.3
1	B	251	ARG	3.2
1	B	78	ASP	3.2
1	B	19	SER	3.1
1	B	273	GLY	3.0
1	B	192	GLU	2.9
1	B	196	ASN	2.9
1	B	265	PHE	2.9
1	B	299	PHE	2.9
1	B	60	THR	2.8
1	A	243	LEU	2.8
1	B	193	GLU	2.7
1	B	56	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	GLU	2.6
1	B	62	VAL	2.6
1	B	191	GLU	2.6
1	B	236	ASN	2.5
1	B	190	THR	2.5
1	B	53	TYR	2.4
1	A	333	ARG	2.3
1	B	188	ASP	2.3
1	A	262	GLN	2.3
1	B	274	TRP	2.3
1	B	54	ASP	2.3
1	B	21	MET	2.1
1	B	55	ARG	2.1
1	B	59	LYS	2.1
1	B	198	LEU	2.0
1	B	291	HIS	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(Å ²)	Q<0.9
2	GOL	B	402	6/6	0.80	0.16	26,37,41,45	6
2	GOL	A	402	6/6	0.88	0.13	34,42,45,45	0
2	GOL	A	401	6/6	0.93	0.09	28,35,36,37	0
2	GOL	B	401	6/6	0.94	0.09	32,36,42,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.