Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 01:36 am BST

PDB ID	:	6B2S
Title	:	Crystal structure of Xanthomonas campestris OleA H285N
Authors	:	Jensen, M.R.; Goblirsch, B.R.; Esler, M.A.; Christenson, J.K.; Mohamed, F.A.; Wackett, L.P.; Wilmot, C.M.
Deposited on	:	2017-09-20
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.226
Clashscore		2
Ramachandran outliers		0.6%
Sidechain outliers		2.2%
RSRZ outliers		5.9%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
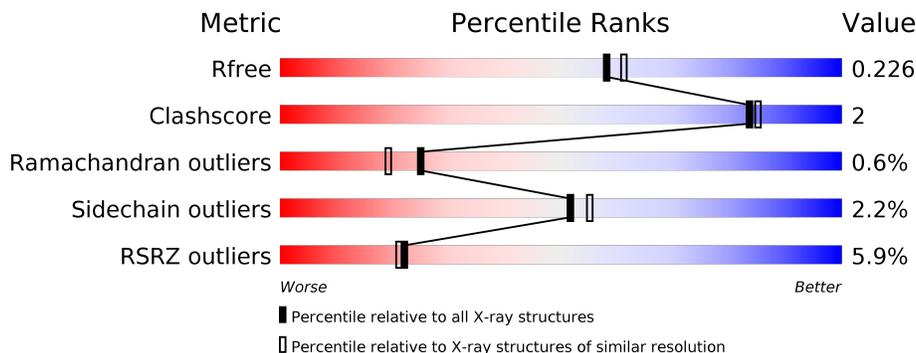
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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 <=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% 87% 9% •
1	B	358	9% 80% 13% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5391 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 2620	C 1645	N 462	O 498	S 15	0	0	0
1	B	339	Total 2596	C 1627	N 456	O 497	S 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	285	ASN	HIS	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	285	ASN	HIS	engineered mutation	UNP Q8PDX2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
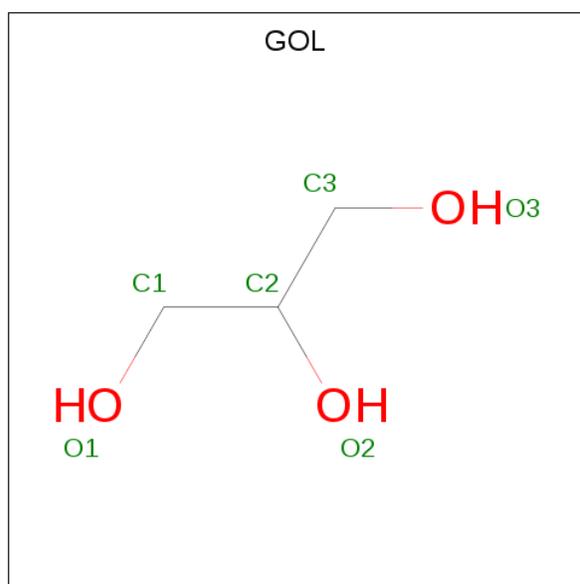
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
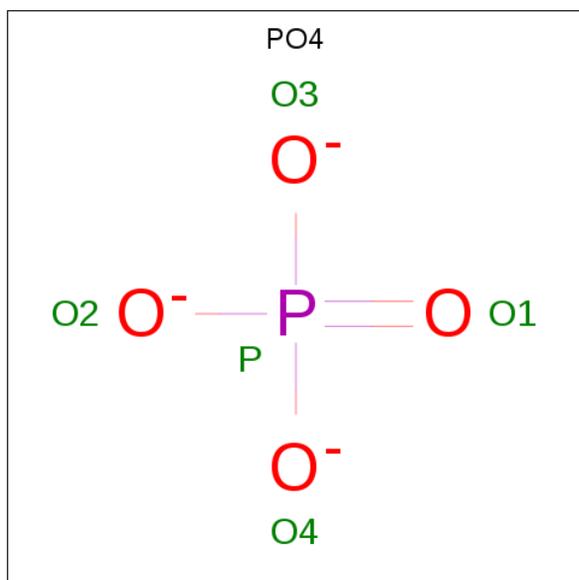
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total 76	O 76	0	0
4	B	49	Total 49	O 49	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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
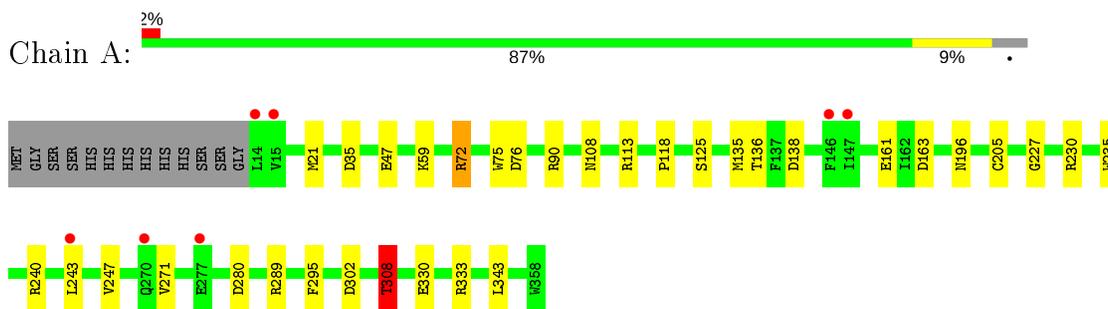
- Molecule 1: 3-oxoacyl-[ACP] synthase III
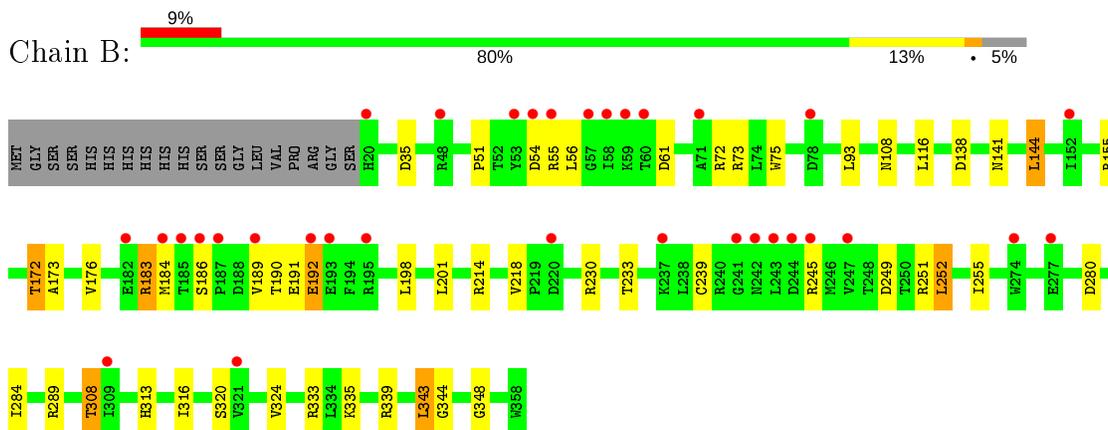
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.52Å 85.08Å 103.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.00 29.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.72-2.00) 98.8 (29.72-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.60 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.164 , 0.218 0.175 , 0.226	Depositor DCC
R_{free} test set	2420 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 51.5	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5391	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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, CSO, 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	1.18	4/2651 (0.2%)	1.20	19/3588 (0.5%)
1	B	1.18	2/2619 (0.1%)	1.20	21/3544 (0.6%)
All	All	1.18	6/5270 (0.1%)	1.20	40/7132 (0.6%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	THR	CB-CG2	-6.05	1.32	1.52
1	A	47	GLU	CD-OE1	5.56	1.31	1.25
1	A	308	THR	CB-CG2	-5.37	1.34	1.52
1	A	235	TRP	CG-CD1	5.27	1.44	1.36
1	A	227	GLY	C-O	-5.10	1.15	1.23
1	B	183	ARG	CD-NE	5.06	1.55	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	B	35	ASP	CB-CG-OD1	10.11	127.40	118.30
1	B	214	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	76	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	59	LYS	CD-CE-NZ	-8.26	92.71	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	B	61	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	289	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	73	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	113	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	230	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	333	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	90	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	214	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	B	339	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	333	ARG	CG-CD-NE	-6.33	98.50	111.80
1	A	35	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	76	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	302	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	245	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	72	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	249	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	339	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	B	172	THR	OG1-CB-CG2	-5.77	96.73	110.00
1	A	135	MET	CG-SD-CE	5.72	109.35	100.20
1	A	90	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	252	LEU	CB-CG-CD2	5.65	120.60	111.00
1	A	230	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	289	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	163	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	280	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	230	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	280	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	333	ARG	CG-CD-NE	5.28	122.88	111.80
1	B	183	ARG	CA-CB-CG	5.21	124.87	113.40
1	B	144	LEU	CB-CA-C	-5.20	100.33	110.20
1	A	308	THR	N-CA-CB	-5.15	100.51	110.30
1	B	245	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	240	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	93	LEU	CB-CG-CD2	5.10	119.66	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	192	GLU	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	2620	0	2661	11	0
1	B	2596	0	2625	18	0
2	A	18	0	24	0	0
2	B	12	0	16	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	76	0	0	1	0
4	B	49	0	0	0	0
All	All	5391	0	5326	25	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 2.

All (25) 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:B:251:ARG:O	1:B:255:ILE:HD12	1.96	0.66
1:B:186:SER:O	1:B:189:VAL:HG23	1.96	0.65
1:B:284:ILE:HG22	1:B:343:LEU:HG	1.78	0.64
1:A:161:GLU:OE2	1:B:155:ARG:NH1	2.33	0.61
1:B:198:LEU:HD23	1:B:201:LEU:HD12	1.88	0.56
1:A:243:LEU:HD23	1:B:116:LEU:HD11	1.89	0.55
1:A:125:SER:OG	1:A:136:THR:HG21	2.09	0.53
1:B:173:ALA:O	1:B:176:VAL:HG12	2.08	0.52
1:B:54:ASP:O	1:B:56:LEU:N	2.45	0.49
1:A:295:PHE:CZ	1:A:343:LEU:HD22	2.47	0.49
1:A:308:THR:HG23	4:A:546:HOH:O	2.16	0.46
1:A:196:ASN:HB3	1:A:247:VAL:HG13	1.99	0.45
1:A:118:PRO:HD3	1:B:239:CYS:O	2.17	0.45
1:B:108:ASN:HB3	1:B:138:ASP:OD1	2.17	0.45
1:B:313:HIS:HB3	1:B:316:ILE:HD11	1.99	0.44
1:A:21:MET:HE2	1:A:21:MET:HB2	1.89	0.44
1:A:161:GLU:CD	1:B:155:ARG:HH12	2.22	0.43
1:B:144:LEU:HD22	1:B:344:GLY:HA3	2.00	0.43
1:B:75:TRP:CD1	1:B:172:THR:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:HA	1:B:348:GLY:O	2.18	0.42
1:A:75:TRP:NE1	1:A:205:CYS:HB3	2.35	0.41
1:B:218:VAL:HG23	1:B:218:VAL:O	2.21	0.41
1:B:184:MET:C	1:B:189:VAL:HG21	2.41	0.40
1:B:320[B]:SER:O	1:B:324:VAL:HG23	2.21	0.40
1:A:108:ASN:HB3	1:A:138:ASP:OD1	2.22	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	342/358 (96%)	332 (97%)	10 (3%)	0	100	100
1	B	338/358 (94%)	319 (94%)	15 (4%)	4 (1%)	13	7
All	All	680/716 (95%)	651 (96%)	25 (4%)	4 (1%)	25	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ARG
1	B	190	THR
1	B	141	ASN
1	B	183	ARG

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	278/289 (96%)	274 (99%)	4 (1%)	67	72
1	B	275/289 (95%)	267 (97%)	8 (3%)	42	43
All	All	553/578 (96%)	541 (98%)	12 (2%)	52	55

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	271	VAL
1	A	308	THR
1	A	330	GLU
1	B	51	PRO
1	B	72	ARG
1	B	191	GLU
1	B	192	GLU
1	B	252	LEU
1	B	308	THR
1	B	335	LYS
1	B	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	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)

3 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	CSO	B	143[A]	1	3,6,7	0.86	0	0,6,8	0.00	-
1	CSO	B	143[B]	1	3,6,7	0.88	0	0,6,8	0.00	-
1	CSO	A	143	1	3,6,7	1.95	1 (33%)	0,6,8	0.00	-

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	CSO	B	143[A]	1	-	0/1/5/7	-
1	CSO	B	143[B]	1	-	1/1/5/7	-
1	CSO	A	143	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	CSO	CB-CA	3.11	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	143[B]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	0.93	0	6,6,6	0.75	0
3	PO4	B	403	-	4,4,4	0.68	0	6,6,6	0.88	0
2	GOL	A	402	-	5,5,5	0.18	0	5,5,5	0.38	0
2	GOL	A	401	-	5,5,5	0.19	0	5,5,5	0.81	0
2	GOL	B	401	-	5,5,5	0.77	0	5,5,5	0.48	0
3	PO4	A	405	-	4,4,4	0.76	0	6,6,6	0.75	0
2	GOL	B	402	-	5,5,5	0.28	0	5,5,5	1.22	1 (20%)
3	PO4	B	404	-	4,4,4	0.71	0	6,6,6	0.81	0
2	GOL	A	403	-	5,5,5	0.40	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	A	402	-	-	4/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	403	-	-	0/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	GOL	O1-C1-C2	-2.11	100.07	110.20

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	A	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	C1-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O2-C2-C3-O3
2	A	402	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 (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	344/358 (96%)	-0.08	7 (2%) 65	63	19, 29, 43, 61	0
1	B	338/358 (94%)	0.41	33 (9%) 7	7	19, 31, 69, 82	0
All	All	682/716 (95%)	0.16	40 (5%) 22	21	19, 30, 61, 82	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	LEU	8.5
1	B	58	ILE	6.1
1	B	187	PRO	5.9
1	B	59	LYS	5.4
1	A	14	LEU	5.4
1	B	78	ASP	4.6
1	B	244	ASP	4.6
1	A	243	LEU	4.1
1	B	53	TYR	3.9
1	B	186	SER	3.7
1	B	247	VAL	3.5
1	B	185	THR	3.4
1	B	277	GLU	3.4
1	B	242	ASN	3.3
1	A	15	VAL	3.3
1	B	193	GLU	3.2
1	B	57	GLY	2.9
1	B	189	VAL	2.8
1	B	245	ARG	2.8
1	A	277	GLU	2.8
1	B	60	THR	2.7
1	B	182	GLU	2.6
1	B	274	TRP	2.6
1	B	20	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLU	2.5
1	A	147	ILE	2.5
1	B	48	ARG	2.5
1	B	309	ILE	2.5
1	B	54	ASP	2.5
1	B	220	ASP	2.5
1	B	184	MET	2.4
1	B	321	VAL	2.4
1	A	270	GLN	2.3
1	B	55	ARG	2.3
1	A	146	PHE	2.3
1	B	195	ARG	2.2
1	B	237	LYS	2.2
1	B	241	GLY	2.1
1	B	152	ILE	2.1
1	B	71	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	B	143[A]	7/8	0.95	0.21	22,24,30,36	7
1	CSO	B	143[B]	7/8	0.95	0.21	22,23,26,30	7
1	CSO	A	143	7/8	0.95	0.18	21,23,32,47	0

6.3 Carbohydrates (i)

There are no carbohydrates 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	0.76	0.35	81,82,86,90	0
2	GOL	A	401	6/6	0.88	0.20	46,46,48,49	0
3	PO4	B	404	5/5	0.89	0.17	56,67,71,76	0
2	GOL	A	402	6/6	0.90	0.22	48,56,65,69	0
2	GOL	B	401	6/6	0.91	0.26	37,38,40,50	0
2	GOL	B	402	6/6	0.91	0.18	46,52,61,61	0
3	PO4	B	403	5/5	0.91	0.26	53,62,66,69	0
3	PO4	A	405	5/5	0.92	0.15	71,75,84,85	0
2	GOL	A	403	6/6	0.95	0.12	34,40,42,45	0

6.5 Other polymers (i)

There are no such residues in this entry.