Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 10:21 AM EDT

PDB ID	:	4HZC
Title	:	Crystal structure of Serine acetyltransferase from Brucella abortus strain S19
Authors	:	Kumar, S.; Samudrala, G.
Deposited on	:	2012-11-15
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 (i) 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 (i)) were used in the production of this report:

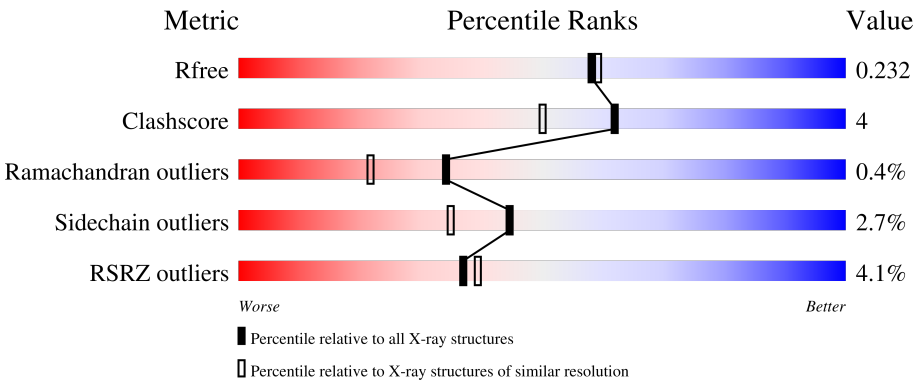
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	281	2%, 80%, 6% •, 13%
1	B	281	2%, 79%, 7%, 13%
1	C	281	%, 81%, 5% •, 13%
1	D	281	3%, 78%, 9%, 13%
1	E	281	2%, 77%, 9%, 14%

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Mol	Chain	Length	Quality of chain
1	F	281	3% 79% 8% 13%
1	G	281	4% 74% 11% • 14%
1	H	281	2% 75% 12% 13%
1	I	281	2% 72% 13% • 13%
1	J	281	9% 70% 16% • 13%
1	K	281	4% 75% 12% 13%
1	L	281	8% 74% 11% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	A	301	-	-	X	-
2	TRS	C	302	-	X	-	-
2	TRS	D	302	-	-	X	-
2	TRS	I	301	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23647 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 CysE, serine acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1879	1187	340	347	5	0	0	0
1	B	244	1874	1184	339	346	5	0	0	0
1	C	245	1879	1187	340	347	5	0	0	0
1	D	245	1879	1187	340	347	5	0	0	0
1	E	243	1870	1182	338	345	5	0	0	0
1	F	245	1877	1186	340	346	5	0	0	0
1	G	242	1862	1178	337	342	5	0	0	0
1	H	245	1877	1187	338	347	5	0	0	0
1	I	244	1869	1181	338	345	5	0	0	0
1	J	244	1868	1181	336	346	5	0	0	0
1	K	245	1875	1184	339	347	5	0	0	0
1	L	245	1883	1190	341	347	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
A	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
A	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
A	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
A	279	HIS	-	EXPRESSION TAG	UNP B2S6A2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
A	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
B	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
B	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
B	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
B	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
B	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
B	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
B	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
C	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
C	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
C	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
C	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
C	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
C	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
C	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
D	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
D	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
D	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
D	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
D	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
D	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
D	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
E	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
E	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
E	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
E	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
E	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
E	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
E	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
F	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
F	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
F	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
F	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
F	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
F	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
F	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
G	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
G	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
G	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
G	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
G	279	HIS	-	EXPRESSION TAG	UNP B2S6A2

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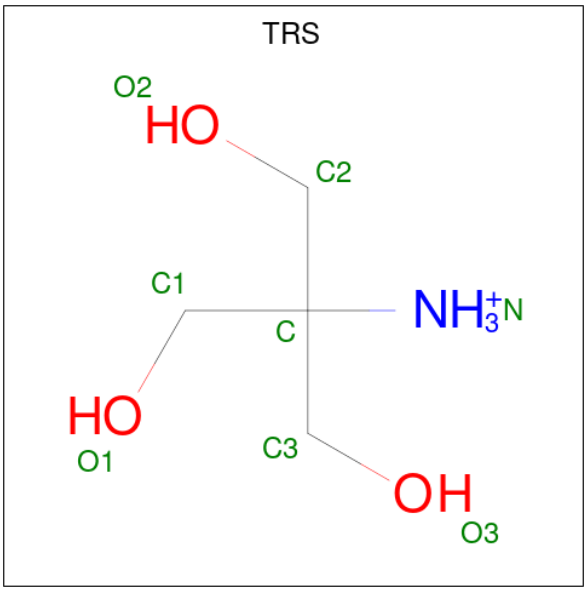
Chain	Residue	Modelled	Actual	Comment	Reference
G	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
G	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
H	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
H	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
H	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
H	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
H	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
H	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
H	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
I	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
I	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
I	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
I	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
I	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
I	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
I	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
J	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
J	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
J	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
J	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
J	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
J	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
J	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
K	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
K	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
K	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
K	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
K	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
K	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
K	281	HIS	-	EXPRESSION TAG	UNP B2S6A2
L	275	LEU	-	EXPRESSION TAG	UNP B2S6A2
L	276	GLU	-	EXPRESSION TAG	UNP B2S6A2
L	277	HIS	-	EXPRESSION TAG	UNP B2S6A2
L	278	HIS	-	EXPRESSION TAG	UNP B2S6A2
L	279	HIS	-	EXPRESSION TAG	UNP B2S6A2
L	280	HIS	-	EXPRESSION TAG	UNP B2S6A2
L	281	HIS	-	EXPRESSION TAG	UNP B2S6A2

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0
2	C	1	8	4	1	3	0	0
2	D	1	8	4	1	3	0	0
2	I	1	8	4	1	3	0	0
2	K	1	8	4	1	3	0	0

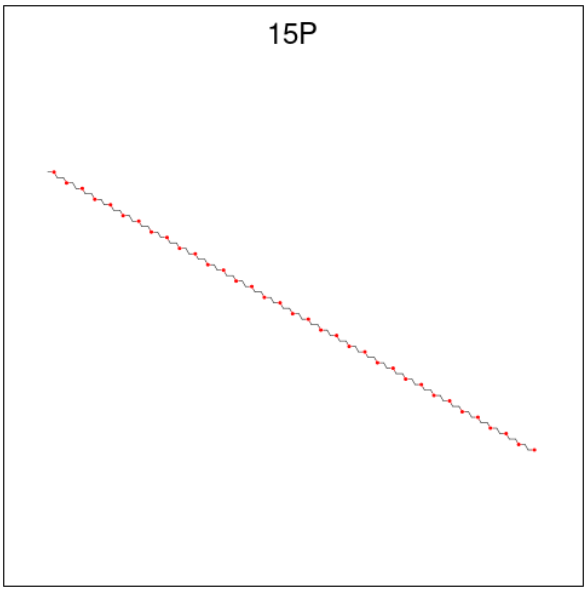
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0
3	J	2	2	2	0	0
3	K	1	1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	G	1	1	1	0	0

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	J	1	10	7	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	129	129	129	0	0
6	B	113	113	113	0	0
6	C	118	118	118	0	0
6	D	112	112	112	0	0
6	E	99	99	99	0	0
6	F	86	86	86	0	0
6	G	80	80	80	0	0

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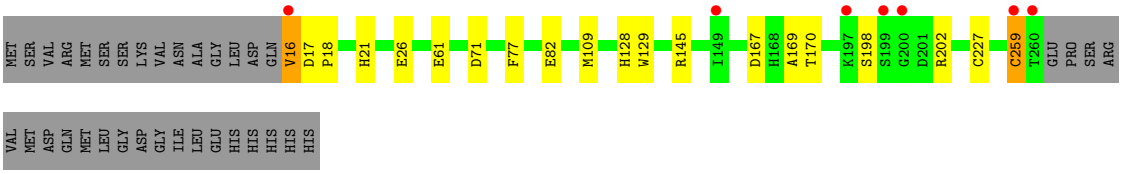
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	89	89	89	0	0
			Total	O		
6	I	87	87	87	0	0
			Total	O		
6	J	57	57	57	0	0
			Total	O		
6	K	76	76	76	0	0
			Total	O		
6	L	49	49	49	0	0

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: CysE, serine acetyltransferase

Chain A:

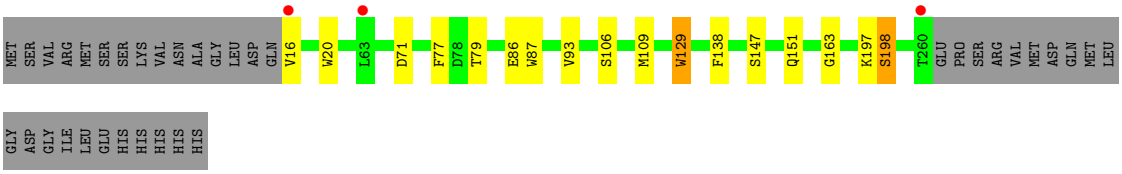


• Molecule 1: CysE, serine acetyltransferase

Chain B:

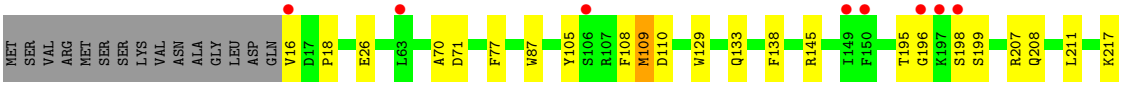
• Molecule 1: CysE, serine acetyltransferase

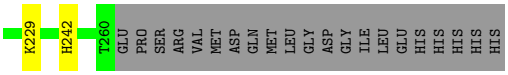
Chain C:



• Molecule 1: CysE, serine acetyltransferase

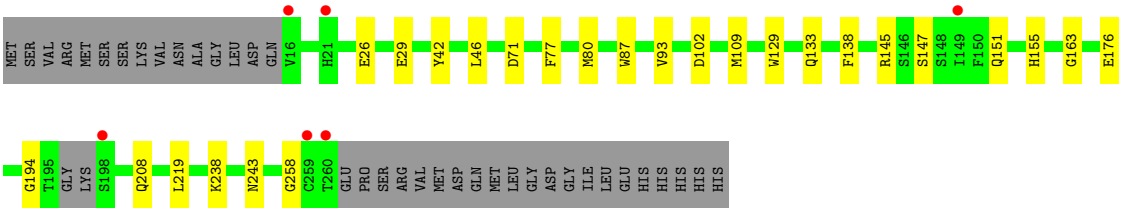
Chain D:





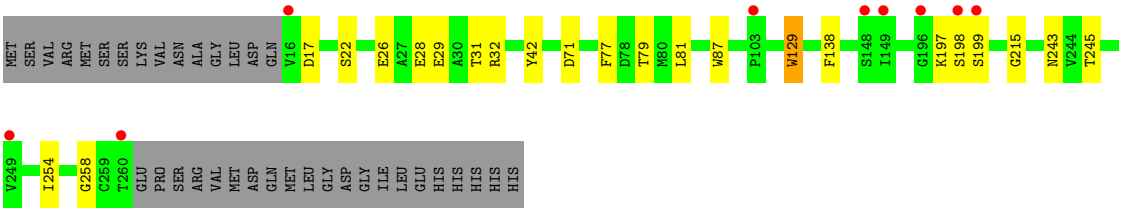
• Molecule 1: CysE, serine acetyltransferase

Chain E:



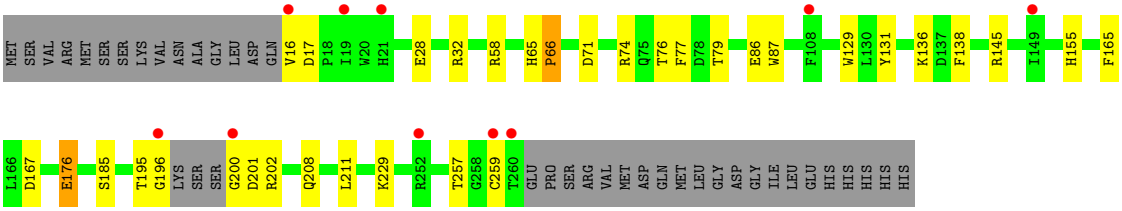
• Molecule 1: CysE, serine acetyltransferase

Chain F:



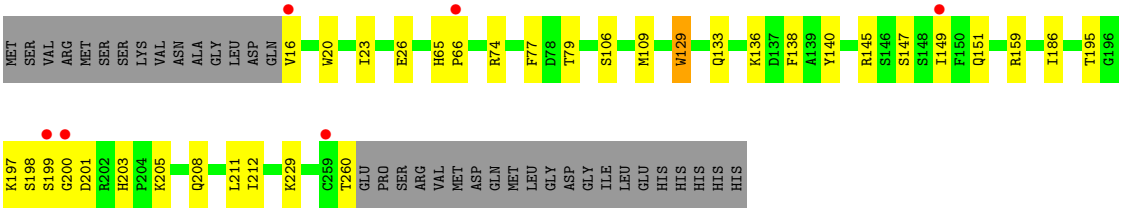
• Molecule 1: CysE, serine acetyltransferase

Chain G:



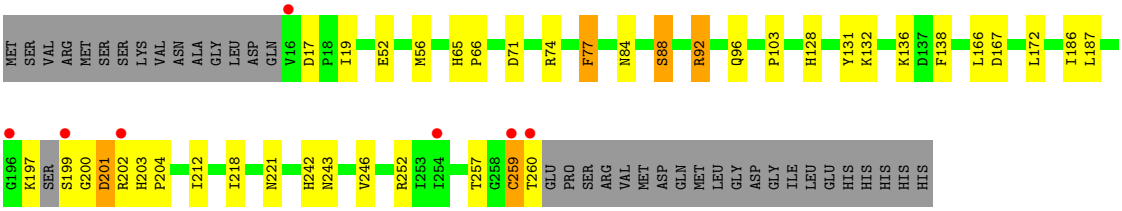
• Molecule 1: CysE, serine acetyltransferase

Chain H:



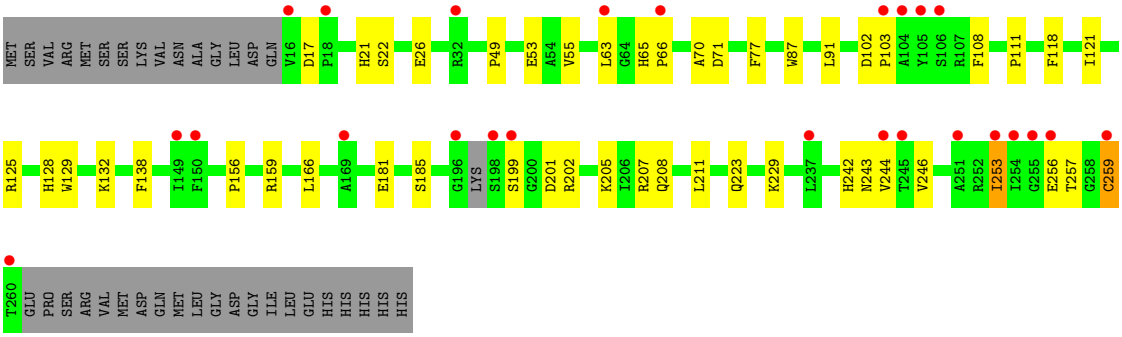
• Molecule 1: CysE, serine acetyltransferase

Chain I:



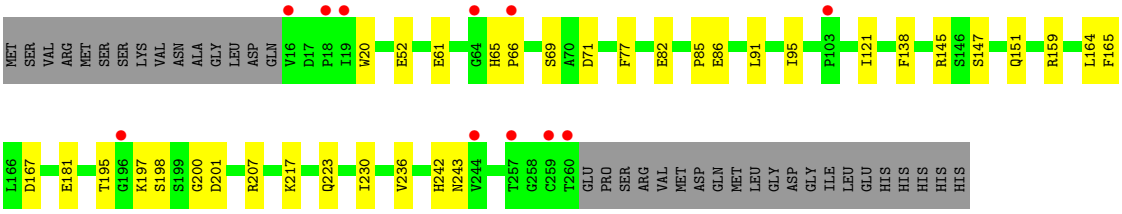
• Molecule 1: CysE, serine acetyltransferase

Chain J:



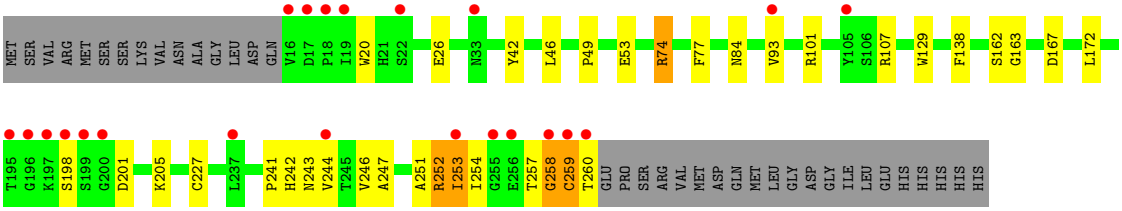
• Molecule 1: CysE, serine acetyltransferase

Chain K:



• Molecule 1: CysE, serine acetyltransferase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.70Å 256.77Å 82.28Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	50.00 – 1.97 46.55 – 1.97	Depositor EDS
% Data completeness (in resolution range)	85.5 (50.00-1.97) 82.8 (46.55-1.97)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.239 0.181 , 0.232	Depositor DCC
R_{free} test set	9193 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23647	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TRS, MG, 15P, CL

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	0.95	2/1921 (0.1%)	0.85	3/2613 (0.1%)
1	B	0.92	2/1915 (0.1%)	0.84	1/2603 (0.0%)
1	C	0.89	3/1921 (0.2%)	0.84	1/2613 (0.0%)
1	D	0.90	1/1921 (0.1%)	0.87	3/2613 (0.1%)
1	E	0.91	1/1911 (0.1%)	0.84	3/2598 (0.1%)
1	F	0.85	1/1919 (0.1%)	0.81	1/2610 (0.0%)
1	G	0.87	2/1903 (0.1%)	0.84	3/2587 (0.1%)
1	H	0.83	2/1919 (0.1%)	0.78	0/2610
1	I	0.81	0/1910	0.84	3/2598 (0.1%)
1	J	0.78	2/1909 (0.1%)	0.81	1/2596 (0.0%)
1	K	0.81	1/1917 (0.1%)	0.78	1/2609 (0.0%)
1	L	0.76	2/1925 (0.1%)	0.85	4/2617 (0.2%)
All	All	0.86	19/22991 (0.1%)	0.83	24/31267 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	TRP	CD2-CE2	6.88	1.49	1.41
1	J	87	TRP	CD2-CE2	6.61	1.49	1.41
1	G	129	TRP	CD2-CE2	6.29	1.49	1.41
1	C	20	TRP	CD2-CE2	6.12	1.48	1.41
1	C	129	TRP	CD2-CE2	5.97	1.48	1.41
1	E	87	TRP	CD2-CE2	5.96	1.48	1.41
1	F	129	TRP	CD2-CE2	5.95	1.48	1.41
1	C	87	TRP	CD2-CE2	5.88	1.48	1.41
1	J	129	TRP	CD2-CE2	5.86	1.48	1.41
1	D	87	TRP	CD2-CE2	5.79	1.48	1.41
1	H	129	TRP	CD2-CE2	5.64	1.48	1.41
1	K	20	TRP	CD2-CE2	5.58	1.48	1.41
1	L	129	TRP	CD2-CE2	5.55	1.48	1.41
1	A	128	HIS	CG-CD2	5.35	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	TRP	CD2-CE2	5.32	1.47	1.41
1	L	20	TRP	CD2-CE2	5.22	1.47	1.41
1	B	20	TRP	CD2-CE2	5.13	1.47	1.41
1	G	87	TRP	CD2-CE2	5.10	1.47	1.41
1	H	20	TRP	CD2-CE2	5.02	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	145	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	L	74	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	I	74	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	L	74	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	E	145	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	D	109	MET	CG-SD-CE	6.85	111.17	100.20
1	G	58	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	A	167	ASP	CB-CG-OD1	6.55	124.19	118.30
1	I	74	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	109	MET	CG-SD-CE	6.20	110.12	100.20
1	C	109	MET	CG-SD-CE	5.79	109.47	100.20
1	F	17	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	145	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	J	125	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	L	167	ASP	CB-CG-OD1	5.55	123.29	118.30
1	E	102	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	167	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	G	145	ARG	CG-CD-NE	-5.37	100.51	111.80
1	A	17	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	207	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	K	145	ARG	CG-CD-NE	-5.04	101.21	111.80
1	L	101	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	I	92	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	E	80	MET	CG-SD-CE	5.00	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

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	1879	0	1861	11	0
1	B	1874	0	1858	14	0
1	C	1879	0	1861	13	0
1	D	1879	0	1861	17	0
1	E	1870	0	1855	11	0
1	F	1877	0	1856	9	0
1	G	1862	0	1848	21	0
1	H	1877	0	1861	16	0
1	I	1869	0	1844	23	0
1	J	1868	0	1847	29	0
1	K	1875	0	1850	19	0
1	L	1883	0	1872	20	0
2	A	8	0	11	7	0
2	C	8	0	12	3	0
2	D	8	0	12	7	0
2	I	8	0	12	4	0
2	K	8	0	12	4	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
4	G	1	0	0	1	0
5	J	10	0	10	2	0
6	A	129	0	0	2	0
6	B	113	0	0	0	0
6	C	118	0	0	0	0
6	D	112	0	0	2	0
6	E	99	0	0	0	0
6	F	86	0	0	0	0
6	G	80	0	0	2	0
6	H	89	0	0	1	0
6	I	87	0	0	1	0
6	J	57	0	0	2	0
6	K	76	0	0	0	0
6	L	49	0	0	1	0
All	All	23647	0	22343	196	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 (196) 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:D:70:ALA:HB3	2:D:302:TRS:H21	1.37	1.04
2:A:301:TRS:H32	1:B:71:ASP:OD2	1.57	1.01
1:A:198:SER:HB2	1:A:202:ARG:HD2	1.41	1.00
2:D:302:TRS:H32	1:E:71:ASP:OD2	1.66	0.96
1:C:197:LYS:N	1:C:198:SER:HB2	1.84	0.91
1:C:71:ASP:OD2	2:C:302:TRS:H32	1.70	0.91
1:J:253:ILE:H	1:J:253:ILE:HD12	1.38	0.87
1:C:106:SER:HB3	1:G:201:ASP:HB3	1.56	0.87
1:I:19:ILE:HD13	6:I:449:HOH:O	1.78	0.82
1:C:197:LYS:H	1:C:198:SER:HB2	1.43	0.82
1:G:76:THR:O	1:G:79:THR:HG22	1.82	0.80
1:D:198:SER:O	1:D:199:SER:HB3	1.83	0.77
1:L:49:PRO:HG2	1:L:53:GLU:HG3	1.65	0.77
1:D:195:THR:H	1:D:196:GLY:HA3	1.52	0.74
2:A:301:TRS:C3	1:B:71:ASP:OD2	2.35	0.74
1:J:166:LEU:HG	6:J:454:HOH:O	1.88	0.73
1:J:17:ASP:H	1:J:21:HIS:HE1	1.38	0.72
2:I:301:TRS:H12	1:J:70:ALA:HB3	1.71	0.71
1:L:247:ALA:O	1:L:252:ARG:N	2.22	0.70
1:B:201:ASP:HB3	1:H:106:SER:CB	2.22	0.69
1:I:201:ASP:O	1:I:221:ASN:ND2	2.20	0.69
1:J:17:ASP:H	1:J:21:HIS:CE1	2.11	0.69
1:I:52:GLU:OE2	1:I:88:SER:OG	2.11	0.68
1:L:258:GLY:C	1:L:260:THR:H	1.94	0.68
1:I:103:PRO:HG3	1:K:198:SER:HB2	1.75	0.68
1:A:71:ASP:OD1	2:A:301:TRS:H22	1.96	0.65
1:K:197:LYS:CB	1:K:198:SER:HA	2.27	0.65
1:J:199:SER:HA	1:J:202:ARG:HD3	1.77	0.64
1:B:201:ASP:HB3	1:H:106:SER:HB3	1.80	0.63
1:C:106:SER:HB3	1:G:201:ASP:CB	2.28	0.63
1:G:71:ASP:OD2	2:K:302:TRS:H31	1.98	0.62
1:G:28:GLU:HG3	1:G:32:ARG:NH1	2.14	0.62
1:K:61:GLU:OE2	2:K:302:TRS:O2	2.18	0.62
1:K:159:ARG:HG3	1:K:159:ARG:HH11	1.64	0.62
1:D:195:THR:N	1:D:196:GLY:HA3	2.11	0.62
1:L:42:TYR:HA	1:L:46:LEU:HB2	1.82	0.62
1:D:217:LYS:HE3	1:F:215:GLY:HA3	1.82	0.62
1:G:79:THR:HG21	6:G:438:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:246:VAL:CG1	1:L:251:ALA:HB1	2.31	0.61
1:A:21:HIS:HD2	6:A:497:HOH:O	1.84	0.61
1:G:71:ASP:OD1	2:K:302:TRS:H22	2.00	0.61
1:D:71:ASP:OD2	2:D:302:TRS:H11	2.02	0.60
1:B:86:GLU:H	1:B:86:GLU:CD	2.05	0.59
1:J:185:SER:HB2	1:J:211:LEU:HD12	1.85	0.58
1:F:243:ASN:OD1	1:F:258:GLY:HA2	2.03	0.58
1:J:128:HIS:HD2	1:J:156:PRO:O	1.86	0.58
1:D:70:ALA:CB	2:D:302:TRS:H21	2.23	0.58
1:G:74:ARG:HD3	4:G:301:CL:CL	2.41	0.58
1:L:253:ILE:HD12	1:L:253:ILE:H	1.69	0.58
1:L:93:VAL:HG23	1:L:163:GLY:H	1.68	0.57
1:B:93:VAL:HG23	1:B:163:GLY:H	1.69	0.57
1:A:71:ASP:OD2	2:A:301:TRS:H11	2.05	0.57
1:E:194:GLY:O	1:E:219:LEU:HD22	2.05	0.56
1:C:86:GLU:H	1:C:86:GLU:CD	2.08	0.56
1:C:71:ASP:OD2	2:C:302:TRS:C3	2.50	0.56
1:C:106:SER:CB	1:G:201:ASP:HB3	2.32	0.56
1:I:71:ASP:OD2	2:I:301:TRS:O2	2.23	0.56
1:I:166:LEU:HD21	1:I:172:LEU:HD22	1.88	0.56
1:F:29:GLU:OE1	1:F:32:ARG:NH2	2.38	0.56
1:G:200:GLY:O	1:G:202:ARG:HG2	2.06	0.55
1:K:242:HIS:HD2	1:K:243:ASN:HD22	1.55	0.55
1:F:22:SER:O	1:F:26:GLU:HG3	2.07	0.55
1:I:202:ARG:HB3	1:I:202:ARG:CZ	2.36	0.54
1:J:207:ARG:NE	1:J:223:GLN:OE1	2.40	0.54
1:I:204:PRO:HG2	1:I:218:ILE:O	2.08	0.54
1:I:200:GLY:O	1:I:202:ARG:N	2.41	0.54
1:L:93:VAL:CG2	1:L:162:SER:HB2	2.38	0.54
1:H:145:ARG:O	1:H:149:ILE:HG22	2.08	0.53
1:G:28:GLU:HG3	1:G:32:ARG:HH12	1.74	0.52
1:B:86:GLU:OE1	1:B:86:GLU:N	2.28	0.52
5:J:301:15P:H592	1:K:66:PRO:HG3	1.91	0.51
1:A:198:SER:CB	1:A:202:ARG:HD2	2.27	0.51
1:I:197:LYS:C	1:I:199:SER:OG	2.48	0.51
1:J:108:PHE:O	1:J:111:PRO:HD2	2.11	0.51
1:J:244:VAL:HA	1:J:256:GLU:HA	1.90	0.51
1:K:86:GLU:H	1:K:86:GLU:CD	2.14	0.51
1:L:258:GLY:C	1:L:260:THR:N	2.63	0.50
1:L:241:PRO:HG2	1:L:244:VAL:HG21	1.93	0.50
1:H:79:THR:HG22	1:H:129:TRP:HH2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:GLU:OE2	1:K:207:ARG:NH1	2.38	0.50
1:H:197:LYS:HG2	1:H:198:SER:H	1.75	0.50
1:K:207:ARG:NE	1:K:223:GLN:OE1	2.42	0.50
1:J:128:HIS:CE1	1:J:132:LYS:HE3	2.47	0.49
1:D:211:LEU:HB3	1:D:229:LYS:HG2	1.95	0.49
1:J:17:ASP:O	1:J:21:HIS:ND1	2.46	0.49
1:L:243:ASN:HB3	1:L:257:THR:O	2.12	0.49
1:I:128:HIS:NE2	1:I:132:LYS:HE2	2.28	0.49
2:C:302:TRS:H11	1:F:71:ASP:OD1	2.13	0.49
1:K:147:SER:O	1:K:151:GLN:HA	2.13	0.49
1:H:74:ARG:HD3	6:H:382:HOH:O	2.12	0.48
1:I:65:HIS:CG	1:I:66:PRO:HD2	2.48	0.48
1:K:230:ILE:HD12	1:K:236:VAL:HG21	1.94	0.48
1:E:147:SER:O	1:E:151:GLN:HA	2.13	0.48
1:G:131:TYR:CZ	1:G:136:LYS:HE3	2.49	0.48
1:I:131:TYR:CE1	1:I:136:LYS:HE3	2.48	0.48
1:L:26:GLU:CD	1:L:107:ARG:HB3	2.33	0.48
1:C:93:VAL:HG23	1:C:163:GLY:H	1.79	0.48
1:C:16:VAL:O	1:C:16:VAL:HG13	2.12	0.48
1:H:147:SER:O	1:H:151:GLN:HA	2.13	0.48
1:J:229:LYS:HG3	1:J:257:THR:HG21	1.96	0.48
1:E:26:GLU:OE1	1:E:109:MET:HB2	2.13	0.47
1:J:55:VAL:HG21	1:J:91:LEU:HD11	1.95	0.47
1:L:252:ARG:O	1:L:254:ILE:HG23	2.14	0.47
1:K:52:GLU:HG3	1:K:91:LEU:HD21	1.97	0.47
1:D:195:THR:OG1	1:D:196:GLY:HA3	2.13	0.47
1:H:79:THR:HG22	1:H:129:TRP:CH2	2.49	0.47
1:K:71:ASP:OD1	2:K:302:TRS:H11	2.14	0.47
1:L:93:VAL:HG21	1:L:162:SER:HB2	1.95	0.47
1:I:128:HIS:CD2	1:I:132:LYS:HE2	2.50	0.47
1:J:246:VAL:HG12	1:J:253:ILE:HA	1.97	0.47
1:B:195:THR:HA	1:B:196:GLY:HA2	1.62	0.46
2:I:301:TRS:H31	1:J:71:ASP:OD1	2.14	0.46
1:E:129:TRP:O	1:E:133:GLN:HG2	2.16	0.46
1:L:241:PRO:HG2	1:L:244:VAL:CG2	2.46	0.46
1:K:159:ARG:HG3	1:K:159:ARG:NH1	2.29	0.46
1:J:102:ASP:HA	1:J:103:PRO:HD2	1.75	0.46
1:H:23:ILE:HG23	1:H:109:MET:HG3	1.97	0.46
1:E:238:LYS:HB3	1:E:238:LYS:HE2	1.49	0.45
1:J:159:ARG:HH11	1:J:159:ARG:HG3	1.81	0.45
1:I:71:ASP:OD2	2:I:301:TRS:H32	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASP:HA	1:B:103:PRO:HD3	1.90	0.45
1:J:201:ASP:OD2	1:J:205:LYS:NZ	2.48	0.45
1:E:93:VAL:HG12	1:E:163:GLY:CA	2.47	0.45
1:I:17:ASP:OD2	1:I:92:ARG:NH2	2.49	0.45
1:B:117:GLY:O	1:B:121:ILE:HG13	2.17	0.45
1:J:49:PRO:HG2	1:J:53:GLU:OE2	2.17	0.45
1:L:227:CYS:HB3	1:L:259:CYS:N	2.32	0.45
1:L:242:HIS:ND1	1:L:243:ASN:ND2	2.65	0.45
1:D:129:TRP:O	1:D:133:GLN:HG2	2.17	0.44
1:I:56:MET:HG2	1:I:77:PHE:CD1	2.52	0.44
1:D:242:HIS:HD2	6:D:475:HOH:O	1.99	0.44
1:F:79:THR:HG22	1:F:129:TRP:HH2	1.83	0.44
1:J:159:ARG:HG3	1:J:159:ARG:NH1	2.32	0.44
1:H:211:LEU:HB3	1:H:229:LYS:HG2	2.00	0.44
1:K:91:LEU:O	1:K:95:ILE:HG13	2.18	0.44
2:D:302:TRS:O2	1:E:71:ASP:OD1	2.35	0.44
1:D:18:PRO:HD2	6:D:438:HOH:O	2.18	0.43
1:L:201:ASP:OD2	1:L:205:LYS:NZ	2.39	0.43
1:H:26:GLU:OE1	1:H:109:MET:HB2	2.17	0.43
1:J:242:HIS:HD2	1:J:243:ASN:HD22	1.66	0.43
2:A:301:TRS:O2	1:B:71:ASP:OD1	2.36	0.43
1:D:105:TYR:HB3	1:D:110:ASP:OD2	2.18	0.43
1:G:195:THR:OG1	1:G:196:GLY:N	2.50	0.43
1:C:147:SER:O	1:C:151:GLN:HA	2.18	0.43
1:D:26:GLU:OE1	1:D:109:MET:HB2	2.18	0.43
1:E:155:HIS:CE1	1:E:176:GLU:HG3	2.54	0.43
1:G:185:SER:HB2	1:G:211:LEU:HD22	2.01	0.43
1:C:16:VAL:O	1:C:16:VAL:CG1	2.66	0.43
1:C:79:THR:HG22	1:C:129:TRP:CH2	2.54	0.43
5:J:301:15P:H612	1:K:69:SER:CB	2.48	0.43
1:A:26:GLU:OE1	1:A:109:MET:HB2	2.19	0.43
1:G:65:HIS:CG	1:G:66:PRO:HD2	2.53	0.43
1:G:136:LYS:NZ	6:G:449:HOH:O	2.51	0.43
1:G:165:PHE:CZ	1:G:167:ASP:HB2	2.54	0.43
1:I:167:ASP:HB3	1:I:187:LEU:HG	1.99	0.43
1:D:71:ASP:CG	2:D:302:TRS:H22	2.40	0.42
1:J:118:PHE:HA	1:J:121:ILE:HD12	2.00	0.42
1:F:245:THR:HG23	1:F:254:ILE:HG13	2.01	0.42
1:I:202:ARG:CZ	1:I:202:ARG:CB	2.98	0.42
1:I:259:CYS:HB3	1:I:260:THR:H	1.62	0.42
1:J:65:HIS:CG	1:J:66:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG13	1:A:18:PRO:HD3	2.00	0.42
1:I:243:ASN:HB3	1:I:257:THR:O	2.19	0.42
1:A:169:ALA:O	1:A:170:THR:C	2.58	0.42
1:D:70:ALA:HB3	2:D:302:TRS:C2	2.28	0.42
1:I:186:ILE:HG12	1:I:212:ILE:HD12	2.02	0.42
1:K:65:HIS:CG	1:K:66:PRO:HD2	2.55	0.42
1:L:252:ARG:HA	1:L:252:ARG:HD3	1.66	0.42
1:E:243:ASN:HD22	1:E:258:GLY:HA2	1.85	0.42
1:A:145:ARG:NH1	6:A:433:HOH:O	2.49	0.42
1:H:186:ILE:HG12	1:H:212:ILE:HD12	2.02	0.42
1:G:155:HIS:HB3	1:G:176:GLU:HA	2.02	0.41
1:J:128:HIS:CD2	1:J:156:PRO:O	2.70	0.41
1:H:136:LYS:HB3	1:H:140:TYR:CE2	2.55	0.41
1:J:63:LEU:HD23	1:J:63:LEU:HA	1.92	0.41
1:A:61:GLU:OE2	2:A:301:TRS:O2	2.38	0.41
1:K:165:PHE:CZ	1:K:167:ASP:HB2	2.55	0.41
1:G:229:LYS:HG3	1:G:257:THR:HG21	2.02	0.41
2:A:301:TRS:H32	1:B:71:ASP:CG	2.35	0.41
1:D:16:VAL:HG13	1:D:16:VAL:O	2.20	0.41
1:F:31:THR:HG21	1:F:42:TYR:HE1	1.86	0.41
1:B:129:TRP:O	1:B:133:GLN:HG2	2.19	0.41
1:B:159:ARG:NH1	1:B:159:ARG:HG3	2.36	0.41
1:G:86:GLU:H	1:G:86:GLU:CD	2.24	0.41
1:H:65:HIS:CG	1:H:66:PRO:HD2	2.56	0.41
1:H:129:TRP:O	1:H:133:GLN:HG2	2.20	0.41
1:H:203:HIS:O	1:H:205:LYS:NZ	2.53	0.41
1:G:16:VAL:HG13	1:G:17:ASP:H	1.85	0.41
1:I:203:HIS:HA	1:I:204:PRO:HD3	1.82	0.41
1:J:181:GLU:HB3	6:J:445:HOH:O	2.20	0.40
1:A:227:CYS:HB3	1:A:259:CYS:HB3	1.82	0.40
1:E:42:TYR:HA	1:E:46:LEU:HB2	2.02	0.40
1:K:121:ILE:HG12	1:K:164:LEU:HD23	2.03	0.40
1:L:74:ARG:HD2	6:L:334:HOH:O	2.20	0.40
1:J:22:SER:O	1:J:26:GLU:HG3	2.21	0.40
1:F:81:LEU:HD13	1:F:87:TRP:HE3	1.87	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	243/281 (86%)	233 (96%)	10 (4%)	0	100	100
1	B	240/281 (85%)	232 (97%)	8 (3%)	0	100	100
1	C	243/281 (86%)	235 (97%)	7 (3%)	1 (0%)	34	22
1	D	243/281 (86%)	232 (96%)	11 (4%)	0	100	100
1	E	239/281 (85%)	230 (96%)	9 (4%)	0	100	100
1	F	243/281 (86%)	231 (95%)	10 (4%)	2 (1%)	19	9
1	G	238/281 (85%)	232 (98%)	6 (2%)	0	100	100
1	H	243/281 (86%)	232 (96%)	9 (4%)	2 (1%)	19	9
1	I	240/281 (85%)	230 (96%)	8 (3%)	2 (1%)	19	9
1	J	240/281 (85%)	228 (95%)	11 (5%)	1 (0%)	34	22
1	K	243/281 (86%)	228 (94%)	14 (6%)	1 (0%)	34	22
1	L	243/281 (86%)	230 (95%)	11 (4%)	2 (1%)	19	9
All	All	2898/3372 (86%)	2773 (96%)	114 (4%)	11 (0%)	34	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	201	ASP
1	I	259	CYS
1	H	199	SER
1	F	198	SER
1	J	259	CYS
1	L	259	CYS
1	C	198	SER
1	F	197	LYS
1	H	200	GLY
1	L	258	GLY
1	K	200	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	198/231 (86%)	194 (98%)	4 (2%)	55	48
1	B	198/231 (86%)	194 (98%)	4 (2%)	55	48
1	C	198/231 (86%)	196 (99%)	2 (1%)	76	73
1	D	198/231 (86%)	194 (98%)	4 (2%)	55	48
1	E	198/231 (86%)	194 (98%)	4 (2%)	55	48
1	F	197/231 (85%)	193 (98%)	4 (2%)	55	48
1	G	196/231 (85%)	190 (97%)	6 (3%)	40	28
1	H	198/231 (86%)	190 (96%)	8 (4%)	31	19
1	I	196/231 (85%)	188 (96%)	8 (4%)	30	18
1	J	197/231 (85%)	192 (98%)	5 (2%)	47	39
1	K	197/231 (85%)	190 (96%)	7 (4%)	35	23
1	L	199/231 (86%)	192 (96%)	7 (4%)	36	24
All	All	2370/2772 (86%)	2307 (97%)	63 (3%)	44	35

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	77	PHE
1	A	82	GLU
1	A	259	CYS
1	B	28	GLU
1	B	77	PHE
1	B	138	PHE
1	B	260	THR
1	C	77	PHE
1	C	138	PHE
1	D	77	PHE
1	D	108	PHE
1	D	138	PHE
1	D	208	GLN

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Mol	Chain	Res	Type
1	E	29	GLU
1	E	77	PHE
1	E	138	PHE
1	E	208	GLN
1	F	28	GLU
1	F	77	PHE
1	F	138	PHE
1	F	199	SER
1	G	66	PRO
1	G	77	PHE
1	G	138	PHE
1	G	176	GLU
1	G	208	GLN
1	G	259	CYS
1	H	16	VAL
1	H	77	PHE
1	H	138	PHE
1	H	159	ARG
1	H	195	THR
1	H	201	ASP
1	H	208	GLN
1	H	260	THR
1	I	77	PHE
1	I	84	ASN
1	I	88	SER
1	I	96	GLN
1	I	138	PHE
1	I	242	HIS
1	I	246	VAL
1	I	252	ARG
1	J	77	PHE
1	J	138	PHE
1	J	208	GLN
1	J	253	ILE
1	J	259	CYS
1	K	77	PHE
1	K	82	GLU
1	K	85	PRO
1	K	138	PHE
1	K	195	THR
1	K	201	ASP
1	K	217	LYS

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Mol	Chain	Res	Type
1	L	77	PHE
1	L	84	ASN
1	L	138	PHE
1	L	172	LEU
1	L	198	SER
1	L	252	ARG
1	L	253	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	243	ASN
1	J	21	HIS
1	J	128	HIS
1	J	243	ASN
1	K	183	ASN
1	K	243	ASN
1	L	208	GLN
1	L	243	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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	TRS	D	302	-	7,7,7	0.74	0	9,9,9	1.16	1 (11%)
2	TRS	K	302	-	7,7,7	1.23	1 (14%)	9,9,9	1.47	3 (33%)
2	TRS	A	301	-	7,7,7	1.63	2 (28%)	9,9,9	1.70	2 (22%)
5	15P	J	301	-	9,9,103	0.85	0	8,8,102	0.79	0
2	TRS	I	301	-	7,7,7	0.83	0	9,9,9	1.31	2 (22%)
2	TRS	C	302	3	7,7,7	1.36	2 (28%)	9,9,9	1.95	3 (33%)

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	TRS	D	302	-	-	5/9/9/9	-
2	TRS	K	302	-	-	3/9/9/9	-
2	TRS	A	301	-	-	5/9/9/9	-
5	15P	J	301	-	-	4/7/7/101	-
2	TRS	I	301	-	-	9/9/9/9	-
2	TRS	C	302	3	-	9/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	TRS	O2-C2	-3.56	1.30	1.42
2	C	302	TRS	O3-C3	2.48	1.50	1.42
2	K	302	TRS	O3-C3	2.40	1.50	1.42
2	A	301	TRS	C1-C	-2.18	1.47	1.53
2	C	302	TRS	C-N	2.04	1.56	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	TRS	O3-C3-C	-3.89	100.04	110.88
2	A	301	TRS	C3-C-N	3.03	115.89	108.17
2	A	301	TRS	C3-C-C1	-2.77	103.27	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	302	TRS	C2-C-N	-2.74	101.19	108.17
2	C	302	TRS	C2-C-N	2.70	115.06	108.17
2	I	301	TRS	C2-C-N	-2.60	101.53	108.17
2	K	302	TRS	O3-C3-C	-2.45	104.05	110.88
2	K	302	TRS	C2-C-C1	-2.16	104.91	110.66
2	I	301	TRS	C3-C-N	2.05	113.40	108.17
2	K	302	TRS	C2-C-N	2.02	113.33	108.17
2	C	302	TRS	O2-C2-C	2.02	116.51	110.88

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TRS	C1-C-C2-O2
2	A	301	TRS	C3-C-C2-O2
2	A	301	TRS	N-C-C2-O2
2	C	302	TRS	C1-C-C2-O2
2	C	302	TRS	C3-C-C2-O2
2	C	302	TRS	N-C-C2-O2
2	D	302	TRS	N-C-C2-O2
2	D	302	TRS	N-C-C3-O3
2	I	301	TRS	C1-C-C2-O2
2	I	301	TRS	C3-C-C2-O2
2	I	301	TRS	N-C-C2-O2
2	I	301	TRS	C1-C-C3-O3
2	I	301	TRS	C2-C-C3-O3
2	I	301	TRS	N-C-C3-O3
2	K	302	TRS	C2-C-C1-O1
2	C	302	TRS	C2-C-C1-O1
2	C	302	TRS	C2-C-C3-O3
2	I	301	TRS	C2-C-C1-O1
5	J	301	15P	O29-C59-C60-O30
2	A	301	TRS	N-C-C1-O1
2	C	302	TRS	N-C-C1-O1
2	C	302	TRS	N-C-C3-O3
2	D	302	TRS	C1-C-C3-O3
2	I	301	TRS	N-C-C1-O1
2	K	302	TRS	N-C-C1-O1
5	J	301	15P	C58-C57-O28-C56
5	J	301	15P	C57-C58-O29-C59
2	C	302	TRS	C3-C-C1-O1
2	C	302	TRS	C1-C-C3-O3

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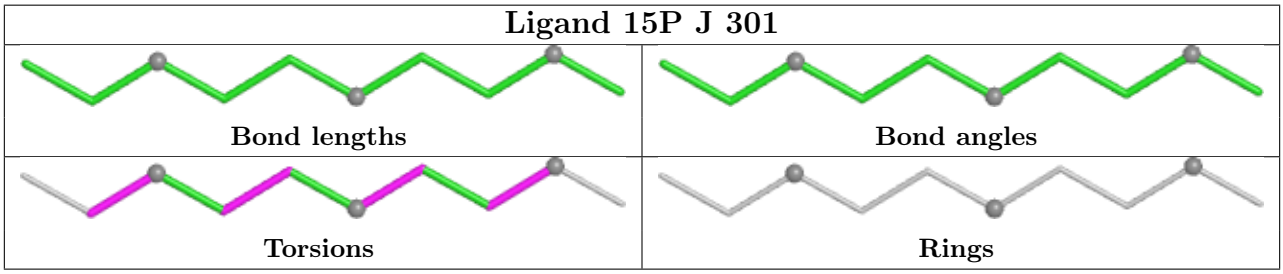
Mol	Chain	Res	Type	Atoms
2	D	302	TRS	C1-C-C2-O2
2	D	302	TRS	C3-C-C2-O2
2	K	302	TRS	C3-C-C1-O1
2	A	301	TRS	C2-C-C1-O1
2	I	301	TRS	C3-C-C1-O1
5	J	301	15P	C62-C61-O30-C60

There are no ring outliers.

6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	TRS	7	0
2	K	302	TRS	4	0
2	A	301	TRS	7	0
5	J	301	15P	2	0
2	I	301	TRS	4	0
2	C	302	TRS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	245/281 (87%)	-0.09	7 (2%)	51	54	17, 26, 45, 74	0
1	B	244/281 (86%)	-0.05	5 (2%)	65	66	18, 29, 49, 88	0
1	C	245/281 (87%)	-0.19	3 (1%)	79	80	19, 28, 44, 70	0
1	D	245/281 (87%)	0.03	8 (3%)	46	49	20, 29, 51, 84	0
1	E	243/281 (86%)	0.02	6 (2%)	57	59	20, 30, 49, 78	0
1	F	245/281 (87%)	0.17	9 (3%)	41	44	19, 35, 56, 89	0
1	G	242/281 (86%)	0.06	10 (4%)	37	39	23, 34, 55, 74	0
1	H	245/281 (87%)	0.05	6 (2%)	59	61	24, 35, 53, 83	0
1	I	244/281 (86%)	0.19	7 (2%)	51	54	26, 39, 66, 88	0
1	J	244/281 (86%)	0.66	25 (10%)	6	7	23, 46, 68, 93	0
1	K	245/281 (87%)	0.17	11 (4%)	33	35	24, 38, 59, 84	0
1	L	245/281 (87%)	0.50	22 (8%)	9	10	27, 47, 71, 90	0
All	All	2932/3372 (86%)	0.13	119 (4%)	37	39	17, 34, 61, 93	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	260	THR	8.0
1	H	199	SER	6.1
1	L	16	VAL	5.8
1	J	260	THR	5.2
1	E	16	VAL	4.8
1	F	260	THR	4.5
1	L	199	SER	4.5
1	B	16	VAL	4.3
1	C	16	VAL	4.3
1	K	259	CYS	4.1
1	A	197	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	16	VAL	4.0
1	I	254	ILE	3.9
1	L	244	VAL	3.9
1	K	260	THR	3.8
1	J	198	SER	3.7
1	G	16	VAL	3.7
1	J	199	SER	3.7
1	B	260	THR	3.7
1	F	198	SER	3.7
1	J	106	SER	3.6
1	J	244	VAL	3.5
1	H	200	GLY	3.5
1	J	105	TYR	3.5
1	D	16	VAL	3.5
1	E	260	THR	3.4
1	A	260	THR	3.4
1	L	197	LYS	3.4
1	G	259	CYS	3.3
1	L	256	GLU	3.3
1	G	260	THR	3.2
1	J	253	ILE	3.2
1	G	196	GLY	3.1
1	L	259	CYS	3.1
1	K	196	GLY	3.0
1	F	196	GLY	2.9
1	L	255	GLY	2.9
1	H	149	ILE	2.9
1	A	200	GLY	2.9
1	D	149	ILE	2.9
1	D	106	SER	2.8
1	K	16	VAL	2.8
1	H	16	VAL	2.8
1	J	169	ALA	2.7
1	J	66	PRO	2.7
1	E	198	SER	2.7
1	J	149	ILE	2.7
1	D	198	SER	2.7
1	I	202	ARG	2.7
1	J	196	GLY	2.6
1	J	18	PRO	2.6
1	D	150	PHE	2.6
1	L	198	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	199	SER	2.6
1	F	103	PRO	2.6
1	K	244	VAL	2.6
1	L	18	PRO	2.5
1	A	16	VAL	2.5
1	F	16	VAL	2.5
1	E	149	ILE	2.5
1	F	149	ILE	2.5
1	K	19	ILE	2.5
1	K	103	PRO	2.5
1	L	258	GLY	2.5
1	I	259	CYS	2.5
1	J	256	GLU	2.5
1	J	251	ALA	2.4
1	G	108	PHE	2.4
1	J	259	CYS	2.4
1	L	196	GLY	2.4
1	A	259	CYS	2.4
1	E	259	CYS	2.4
1	I	199	SER	2.4
1	L	22	SER	2.4
1	J	103	PRO	2.4
1	C	260	THR	2.4
1	H	259	CYS	2.4
1	I	16	VAL	2.4
1	L	93	VAL	2.4
1	J	32	ARG	2.3
1	A	149	ILE	2.3
1	B	196	GLY	2.3
1	J	237	LEU	2.3
1	L	33	ASN	2.3
1	E	21	HIS	2.3
1	H	66	PRO	2.3
1	L	200	GLY	2.3
1	L	19	ILE	2.3
1	L	195	THR	2.2
1	F	199	SER	2.2
1	J	63	LEU	2.2
1	J	150	PHE	2.2
1	D	197	LYS	2.2
1	L	253	ILE	2.2
1	D	63	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	196	GLY	2.2
1	G	19	ILE	2.2
1	J	254	ILE	2.2
1	B	63	LEU	2.2
1	K	18	PRO	2.1
1	I	260	THR	2.1
1	K	64	GLY	2.1
1	J	104	ALA	2.1
1	G	21	HIS	2.1
1	G	149	ILE	2.1
1	A	199	SER	2.1
1	J	255	GLY	2.1
1	L	237	LEU	2.1
1	F	148	SER	2.1
1	L	17	ASP	2.1
1	G	252	ARG	2.1
1	G	200	GLY	2.1
1	L	105	TYR	2.0
1	C	63	LEU	2.0
1	K	257	THR	2.0
1	F	249	VAL	2.0
1	D	196	GLY	2.0
1	K	66	PRO	2.0
1	J	245	THR	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)

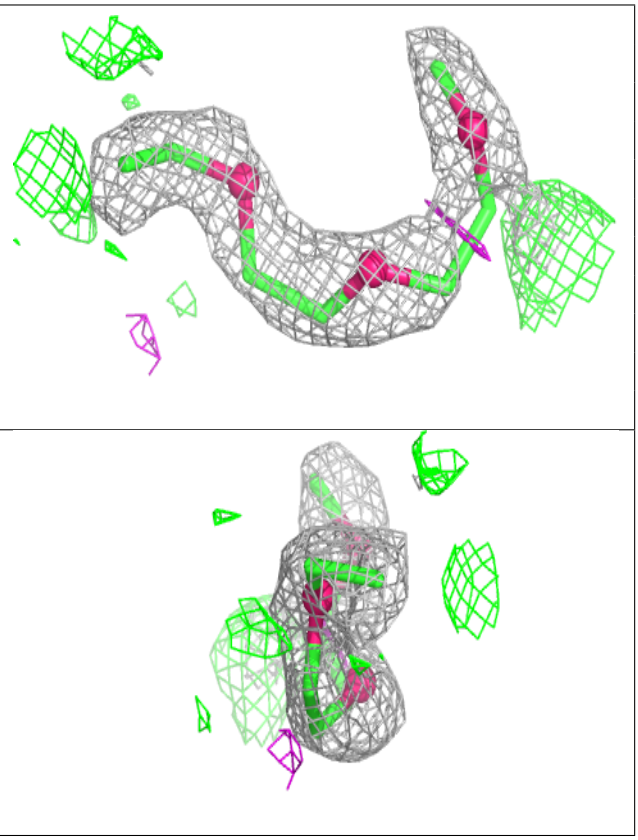
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	15P	J	301	10/104	0.83	0.27	43,55,60,65	0
3	MG	J	302	1/1	0.88	0.26	52,52,52,52	0
2	TRS	D	302	8/8	0.88	0.18	25,34,38,39	0
3	MG	J	303	1/1	0.89	0.26	59,59,59,59	0
2	TRS	K	302	8/8	0.89	0.20	29,33,43,44	0
2	TRS	I	301	8/8	0.90	0.24	34,40,47,59	0
3	MG	D	301	1/1	0.92	0.30	50,50,50,50	0
2	TRS	C	302	8/8	0.92	0.18	23,32,42,45	0
3	MG	G	302	1/1	0.93	0.11	49,49,49,49	0
3	MG	K	301	1/1	0.93	0.10	47,47,47,47	0
2	TRS	A	301	8/8	0.93	0.17	23,31,34,37	0
3	MG	A	303	1/1	0.94	0.10	44,44,44,44	0
3	MG	C	301	1/1	0.95	0.08	40,40,40,40	0
3	MG	F	301	1/1	0.96	0.08	40,40,40,40	0
3	MG	A	302	1/1	0.97	0.14	33,33,33,33	0
4	CL	G	301	1/1	0.99	0.12	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 15P J 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.