Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:10 PM GMT

PDB ID	:	1SET
Title	:	CRYSTAL STRUCTURES AT 2.5 ANGSTROMS RESOLUTION OF SERYL-TRNA SYNTHETASE COMPLEXED WITH TWO DIFFERENT ANALOGUES OF SERYL-ADENYLATE
Authors	:	Cusack, S.; Belrhali, H.
Deposited on	:	1994-02-21
Resolution	:	2.55 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
http://wwpdb.org/validation/2016/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:

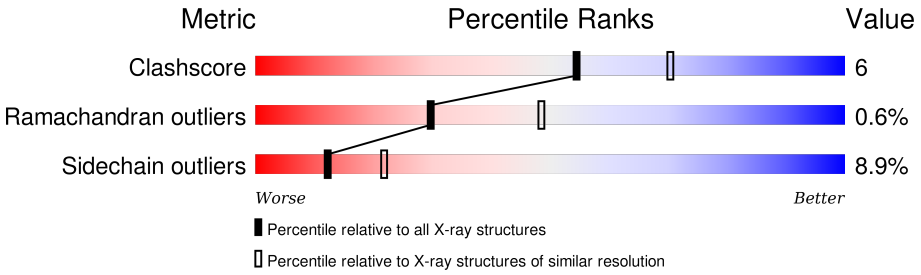
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.55 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))
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	71% 23% 5%
1	B	421	75% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6974 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.

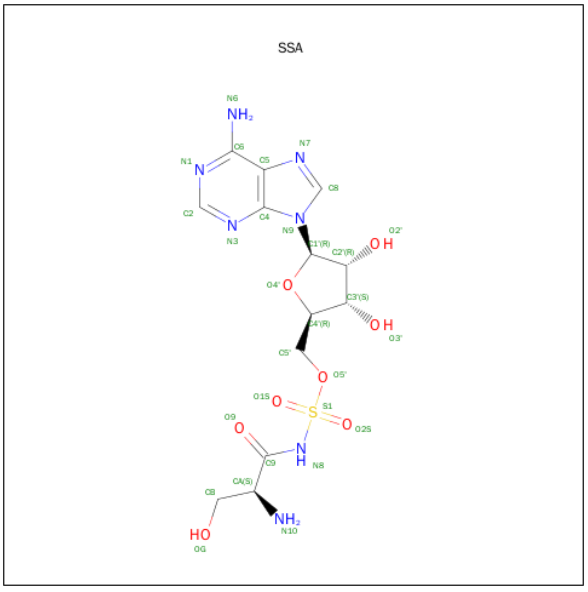
- Molecule 1 is a protein called SERYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	185	0	0
			3373	2143	606	613	11			
1	B	421	Total	C	N	O	S	239	0	0
			3373	2143	606	613	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	CONFLICT	UNP P34945
B	208	TYR	THR	CONFLICT	UNP P34945

- Molecule 2 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (three-letter code: SSA) (formula: $C_{13}H_{19}N_7O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	13	7	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			29	13	7	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	89	Total	O	0	0
			89	89		

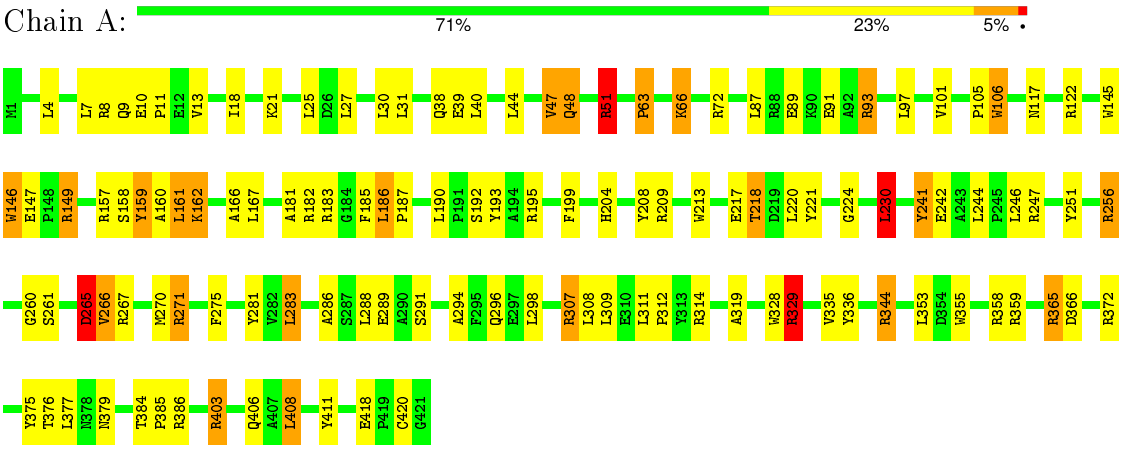
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

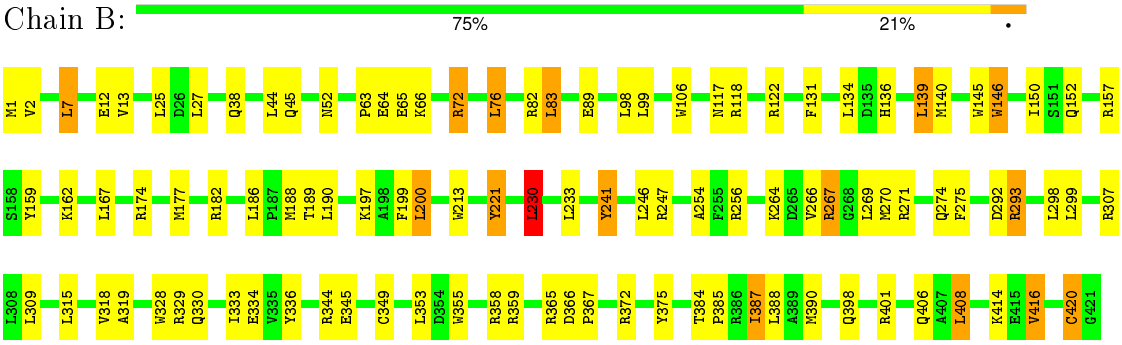
- Molecule 1: SERYL-tRNA SYNTHETASE

Chain A:



- Molecule 1: SERYL-tRNA SYNTHETASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.40Å 126.30Å 62.90Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6974	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SSA

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	0.91	0/3448	1.61	57/4667 (1.2%)
1	B	0.90	0/3448	1.67	64/4667 (1.4%)
All	All	0.90	0/6896	1.64	121/9334 (1.3%)

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

There are no bond length outliers.

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	MET	CG-SD-CE	-17.14	72.77	100.20
1	B	256	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	B	358	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	A	256	ARG	NE-CZ-NH1	11.25	125.93	120.30
1	A	256	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	B	177	MET	CG-SD-CE	-10.60	83.25	100.20
1	B	358	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	256	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	B	118	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	B	106	TRP	CD1-CG-CD2	9.33	113.76	106.30
1	A	403	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	307	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	B	390	MET	CG-SD-CE	8.96	114.54	100.20
1	B	293	ARG	NE-CZ-NH1	8.84	124.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	355	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	B	159	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	B	145	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	B	157	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	359	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	157	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	188	MET	CG-SD-CE	-7.90	87.56	100.20
1	A	307	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	213	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	145	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	B	152	GLN	CA-CB-CG	7.58	130.07	113.40
1	A	372	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	355	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	B	106	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	B	213	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	B	328	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	B	372	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	281	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	A	213	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	106	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	A	106	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	B	146	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	A	162	LYS	CA-CB-CG	6.94	128.67	113.40
1	A	146	TRP	CD1-CG-CD2	6.92	111.84	106.30
1	B	355	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	B	408	LEU	CA-CB-CG	-6.79	99.69	115.30
1	B	213	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	A	329	ARG	CG-CD-NE	-6.74	97.65	111.80
1	A	418	GLU	CA-CB-CG	-6.72	98.61	113.40
1	A	365	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	145	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	344	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	328	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	149	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	146	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	106	TRP	CG-CD1-NE1	-6.46	103.64	110.10
1	B	416	VAL	CG1-CB-CG2	-6.45	100.58	110.90
1	A	195	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	271	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	266	VAL	CA-C-N	-6.37	103.20	117.20
1	A	355	TRP	CE2-CD2-CG	-6.35	102.22	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	271	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	344	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	241	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	B	122	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	318	VAL	CG1-CB-CG2	-6.17	101.03	110.90
1	A	270	MET	CG-SD-CE	-6.15	90.37	100.20
1	B	329	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	139	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	328	TRP	CE2-CD2-CG	-6.07	102.44	107.30
1	B	145	TRP	CE2-CD2-CG	-6.06	102.45	107.30
1	B	146	TRP	CE2-CD2-CG	-6.05	102.46	107.30
1	A	106	TRP	CG-CD2-CE3	6.03	139.33	133.90
1	A	411	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	A	260	GLY	N-CA-C	-5.98	98.15	113.10
1	A	408	LEU	CA-CB-CG	-5.97	101.57	115.30
1	A	72	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	221	TYR	CB-CG-CD2	-5.89	117.46	121.00
1	B	420	CYS	CA-CB-SG	-5.88	103.42	114.00
1	B	270	MET	CG-SD-CE	-5.83	90.87	100.20
1	A	267	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	328	TRP	CD1-CG-CD2	5.80	110.94	106.30
1	A	51	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	256	ARG	CG-CD-NE	-5.74	99.75	111.80
1	A	271	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	267	ARG	N-CA-C	-5.73	95.53	111.00
1	B	387	ILE	CB-CA-C	-5.64	100.32	111.60
1	B	372	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	355	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	265	ASP	CA-C-N	-5.59	104.89	117.20
1	B	145	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	B	336	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	358	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	145	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	A	8	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	146	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	A	244	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	B	307	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	66	LYS	CA-CB-CG	5.43	125.36	113.40
1	B	12	GLU	CA-CB-CG	5.43	125.36	113.40
1	A	365	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	283	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	401	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	B	118	ARG	N-CA-CB	-5.38	100.92	110.60
1	B	267	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	241	TYR	CG-CD2-CE2	-5.37	117.01	121.30
1	B	118	ARG	CA-CB-CG	5.29	125.04	113.40
1	A	328	TRP	CG-CD2-CE3	5.26	138.64	133.90
1	A	72	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	159	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	B	292	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	2	VAL	N-CA-CB	-5.21	100.03	111.50
1	A	230	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	162	LYS	CB-CG-CD	-5.19	98.11	111.60
1	A	372	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	182	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	230	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	146	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	213	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	B	241	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	A	329	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	401	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	146	TRP	CA-CB-CG	5.04	123.28	113.70
1	B	299	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	B	118	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	TYR	Sidechain

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	3373	0	3394	52	9
1	B	3373	0	3394	36	9
2	A	29	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	19	0	0
3	A	81	0	0	0	0
3	B	89	0	0	4	0
All	All	6974	0	6826	82	9

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 6.

All (82) 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:246:LEU:HD12	1:A:283:LEU:HD23	1.72	0.71
1:A:186:LEU:HD11	1:B:162:LYS:HE2	1.71	0.71
1:A:21:LYS:HE3	1:A:105:PRO:HD3	1.77	0.66
1:A:186:LEU:HD21	1:B:420:CYS:SG	2.36	0.64
1:A:190:LEU:HD11	1:A:230:LEU:HD13	1.80	0.63
1:A:157:ARG:HE	1:A:266:VAL:HG21	1.64	0.63
1:A:157:ARG:HH22	1:A:271:ARG:HH21	1.45	0.63
1:A:159:TYR:HD2	1:A:161:LEU:HD13	1.65	0.61
1:B:241:TYR:HB2	1:B:365:ARG:O	2.05	0.57
1:A:157:ARG:NH2	1:A:271:ARG:HH21	2.02	0.57
1:A:117:ASN:ND2	1:A:319:ALA:H	2.03	0.56
1:A:4:LEU:HD23	1:A:7:LEU:HD23	1.87	0.56
1:A:241:TYR:HB2	1:A:365:ARG:O	2.06	0.56
1:B:315:LEU:HD22	1:B:333:ILE:HG12	1.87	0.56
1:B:7:LEU:HD21	1:B:27:LEU:HD11	1.90	0.54
1:B:63:PRO:HA	1:B:66:LYS:HG3	1.90	0.54
1:A:106:TRP:CD1	1:A:329:ARG:HG2	2.42	0.54
1:B:190:LEU:HD11	1:B:230:LEU:HD13	1.90	0.54
1:A:157:ARG:HG2	1:A:266:VAL:HG11	1.90	0.54
1:A:266:VAL:CG2	1:A:271:ARG:HB3	2.38	0.54
1:A:7:LEU:HD11	1:A:27:LEU:HD11	1.90	0.54
1:A:147:GLU:HB3	1:A:160:ALA:HB3	1.90	0.53
1:A:312:PRO:HG2	1:A:336:TYR:HB3	1.91	0.52
1:B:131:PHE:CD2	1:B:398:GLN:HG2	2.45	0.52
1:A:275:PHE:HB2	1:A:384:THR:O	2.10	0.52
1:B:44:LEU:HA	1:B:83:LEU:HD23	1.91	0.51
1:A:193:TYR:HA	1:A:221:TYR:O	2.12	0.50
1:A:192:SER:H	1:B:274:GLN:HE22	1.58	0.50
1:B:334:GLU:HA	1:B:345:GLU:HA	1.94	0.50
1:A:87:LEU:O	1:A:91:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:HIS:HE1	1:B:269:LEU:H	1.59	0.49
1:B:275:PHE:HB2	1:B:384:THR:O	2.11	0.49
1:A:199:PHE:CE2	1:A:221:TYR:HB2	2.47	0.49
1:A:30:LEU:HD12	1:A:97:LEU:HB3	1.94	0.47
1:B:99:LEU:O	1:B:359:ARG:NH2	2.48	0.47
1:A:157:ARG:HE	1:A:266:VAL:HG11	1.80	0.46
1:A:47:VAL:O	1:A:51:ARG:HB2	2.16	0.46
1:A:18:ILE:HD11	1:A:25:LEU:HD23	1.96	0.46
1:B:200:LEU:O	1:B:359:ARG:HD3	2.16	0.46
1:B:414:LYS:HD3	1:B:416:VAL:O	2.16	0.46
1:A:256:ARG:HD3	1:A:275:PHE:HE1	1.81	0.45
1:A:204:HIS:HA	1:A:208:TYR:HD2	1.81	0.45
1:A:25:LEU:HD21	1:A:101:VAL:HG22	1.99	0.45
1:A:158:SER:HA	3:B:429:HOH:O	2.17	0.45
1:B:174:ARG:HA	1:B:174:ARG:HD2	1.88	0.44
1:A:166:ALA:HB1	1:B:189:THR:HG23	1.99	0.44
1:B:174:ARG:HG2	3:B:475:HOH:O	2.17	0.44
1:A:44:LEU:O	1:A:48:GLN:HB2	2.17	0.44
1:A:353:LEU:O	1:A:375:TYR:HA	2.18	0.44
1:A:185:PHE:CD2	1:A:247:ARG:HB3	2.53	0.44
1:A:181:ALA:HB2	1:A:187:PRO:HG3	2.00	0.43
1:B:7:LEU:CD2	1:B:27:LEU:HD11	2.48	0.43
1:B:1:MET:HB2	1:B:359:ARG:CG	2.49	0.43
1:A:89:GLU:HB3	1:A:93:ARG:NH2	2.34	0.43
1:A:122:ARG:HA	1:A:314:ARG:HA	2.01	0.43
1:A:149:ARG:HD3	1:B:233:LEU:O	2.19	0.43
1:B:64:GLU:HG2	1:B:65:GLU:HG3	2.00	0.43
1:B:353:LEU:O	1:B:375:TYR:HA	2.19	0.43
1:B:38:GLN:HG3	3:B:449:HOH:O	2.18	0.42
1:A:294:ALA:HB3	1:A:377:LEU:HD13	2.01	0.42
1:A:311:LEU:HD13	1:A:335:VAL:HG11	2.02	0.42
1:A:218:THR:CG2	1:A:220:LEU:H	2.33	0.42
1:A:283:LEU:HD13	1:A:376:THR:HG22	2.01	0.42
1:A:294:ALA:CB	1:A:377:LEU:HD13	2.49	0.42
1:A:11:PRO:HB3	1:A:31:LEU:HD11	2.01	0.42
1:B:241:TYR:CZ	1:B:367:PRO:HG3	2.55	0.42
1:A:10:GLU:O	1:A:13:VAL:HG22	2.20	0.41
1:A:218:THR:HG22	1:A:220:LEU:H	1.86	0.41
1:B:117:ASN:ND2	1:B:319:ALA:H	2.18	0.41
1:B:365:ARG:HD2	3:B:492:HOH:O	2.20	0.41
1:A:224:GLY:O	1:A:256:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:HD3	1:B:186:LEU:HD21	2.02	0.41
1:B:264:LYS:HE3	1:B:264:LYS:HB2	1.87	0.41
1:A:157:ARG:NE	1:A:266:VAL:HG21	2.32	0.41
1:B:76:LEU:HA	1:B:76:LEU:HD13	1.96	0.41
1:B:385:PRO:O	1:B:388:LEU:HB2	2.21	0.41
1:B:254:ALA:O	1:B:274:GLN:HA	2.21	0.41
1:B:330:GLN:HA	1:B:349:CYS:O	2.20	0.40
1:A:265:ASP:HB2	1:A:344:ARG:NH2	2.36	0.40
1:B:199:PHE:CE2	1:B:221:TYR:HB2	2.56	0.40
1:A:386:ARG:HD3	1:A:386:ARG:HH11	1.74	0.40
1:B:150:ILE:HA	1:B:150:ILE:HD12	1.74	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLN:NE2	1:B:72:ARG:NH2[1_656]	0.70	1.50
1:A:406:GLN:NE2	1:B:72:ARG:CZ[1_656]	0.73	1.47
1:A:406:GLN:CD	1:B:72:ARG:NH2[1_656]	1.04	1.16
1:A:406:GLN:NE2	1:B:72:ARG:NH1[1_656]	1.69	0.51
1:A:406:GLN:CD	1:B:72:ARG:CZ[1_656]	1.84	0.36
1:A:406:GLN:NE2	1:B:72:ARG:NE[1_656]	1.88	0.32
1:A:406:GLN:OE1	1:B:72:ARG:NH2[1_656]	2.02	0.18
1:A:406:GLN:CG	1:B:72:ARG:NH2[1_656]	2.06	0.14
1:A:406:GLN:OE1	1:B:72:ARG:NE[1_656]	2.11	0.09

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	419/421 (100%)	407 (97%)	8 (2%)	4 (1%)	19 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	419/421 (100%)	414 (99%)	4 (1%)	1 (0%)	52 73
All	All	838/842 (100%)	821 (98%)	12 (1%)	5 (1%)	30 48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	B	267	ARG
1	A	261	SER
1	A	286	ALA
1	A	63	PRO

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	347/347 (100%)	312 (90%)	35 (10%)	9 16
1	B	347/347 (100%)	320 (92%)	27 (8%)	16 28
All	All	694/694 (100%)	632 (91%)	62 (9%)	12 22

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	38	GLN
1	A	39	GLU
1	A	40	LEU
1	A	47	VAL
1	A	48	GLN
1	A	51	ARG
1	A	63	PRO
1	A	66	LYS
1	A	146	TRP
1	A	161	LEU

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	182	ARG
1	A	183	ARG
1	A	186	LEU
1	A	209	ARG
1	A	217	GLU
1	A	218	THR
1	A	230	LEU
1	A	242	GLU
1	A	288	LEU
1	A	289	GLU
1	A	291	SER
1	A	296	GLN
1	A	298	LEU
1	A	307	ARG
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	366	ASP
1	A	379	ASN
1	A	385	PRO
1	A	403	ARG
1	A	408	LEU
1	A	420	CYS
1	B	7	LEU
1	B	13	VAL
1	B	25	LEU
1	B	45	GLN
1	B	52	ASN
1	B	72	ARG
1	B	76	LEU
1	B	82	ARG
1	B	83	LEU
1	B	89	GLU
1	B	98	LEU
1	B	134	LEU
1	B	139	LEU
1	B	146	TRP
1	B	167	LEU
1	B	197	LYS
1	B	200	LEU
1	B	230	LEU

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	266	VAL
1	B	293	ARG
1	B	298	LEU
1	B	309	LEU
1	B	366	ASP
1	B	387	ILE
1	B	406	GLN
1	B	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	117	ASN
1	A	280	GLN
1	A	301	ASN
1	A	379	ASN
1	B	117	ASN
1	B	136	HIS
1	B	231	ASN
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	301	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SSA	A	422	-	24,31,31	1.43	3 (12%)	29,46,46	2.01	6 (20%)
2	SSA	B	423	-	24,31,31	1.24	1 (4%)	29,46,46	3.11	8 (27%)

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	SSA	A	422	-	-	0/15/37/37	0/3/3/3
2	SSA	B	423	-	-	0/15/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	422	SSA	C9-N8	-4.57	1.30	1.37
2	B	423	SSA	C9-N8	-3.08	1.32	1.37
2	A	422	SSA	C8-N7	-2.06	1.30	1.34
2	A	422	SSA	O4'-C1'	3.39	1.45	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	423	SSA	O2S-S1-O1S	-13.96	104.04	120.77
2	A	422	SSA	O2S-S1-O1S	-7.63	111.63	120.77
2	B	423	SSA	C5'-O5'-S1	-3.28	111.73	118.02
2	B	423	SSA	OG-CB-CA	-2.72	105.35	111.16
2	A	422	SSA	O2S-S1-N8	-2.38	105.31	108.50
2	B	423	SSA	CA-C9-N8	-2.03	110.75	114.85
2	B	423	SSA	C4-C5-N7	2.19	111.50	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	422	SSA	O4'-C4'-C5'	2.46	118.11	109.32
2	A	422	SSA	O9-C9-N8	2.58	126.14	121.62
2	B	423	SSA	O5'-S1-O1S	2.61	113.75	105.66
2	A	422	SSA	O4'-C1'-N9	2.73	113.81	108.10
2	A	422	SSA	O5'-S1-O1S	2.76	114.23	105.66
2	B	423	SSA	O9-C9-N8	3.79	128.25	121.62
2	B	423	SSA	O2S-S1-N8	4.40	114.37	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.