



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 2CJB / pdb_00002cjb
Title : Crystal structure of Methanosarcina barkeri seryl-tRNA synthetase complexed with serine
Authors : Bilokapic, S.; Maier, T.; Ahel, D.; Gruic-Sovulj, I.; Soll, D.; Weygand-Durasevic, I.; Ban, N.
Deposited on : 2006-03-30
Resolution : 2.70 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

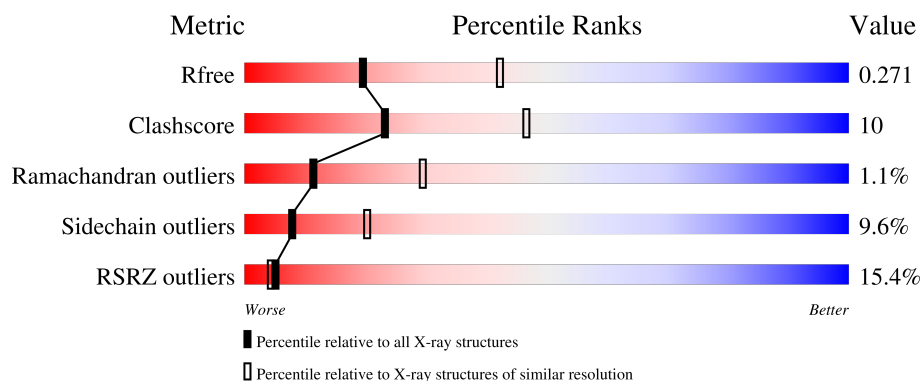
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	522	24% 65% 22% • 9%
1	B	522	5% 68% 23% • 5%

2 Entry composition [i](#)

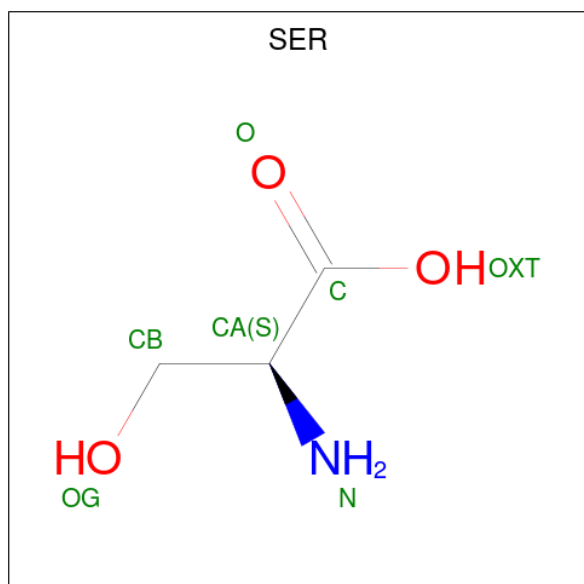
There are 5 unique types of molecules in this entry. The entry contains 8045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	474	Total	C	N	O	S	0	1	0
			3886	2495	660	710	21			
1	B	495	Total	C	N	O	S	0	1	0
			4042	2596	688	737	21			

- Molecule 2 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	3	1	3		
2	B	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0

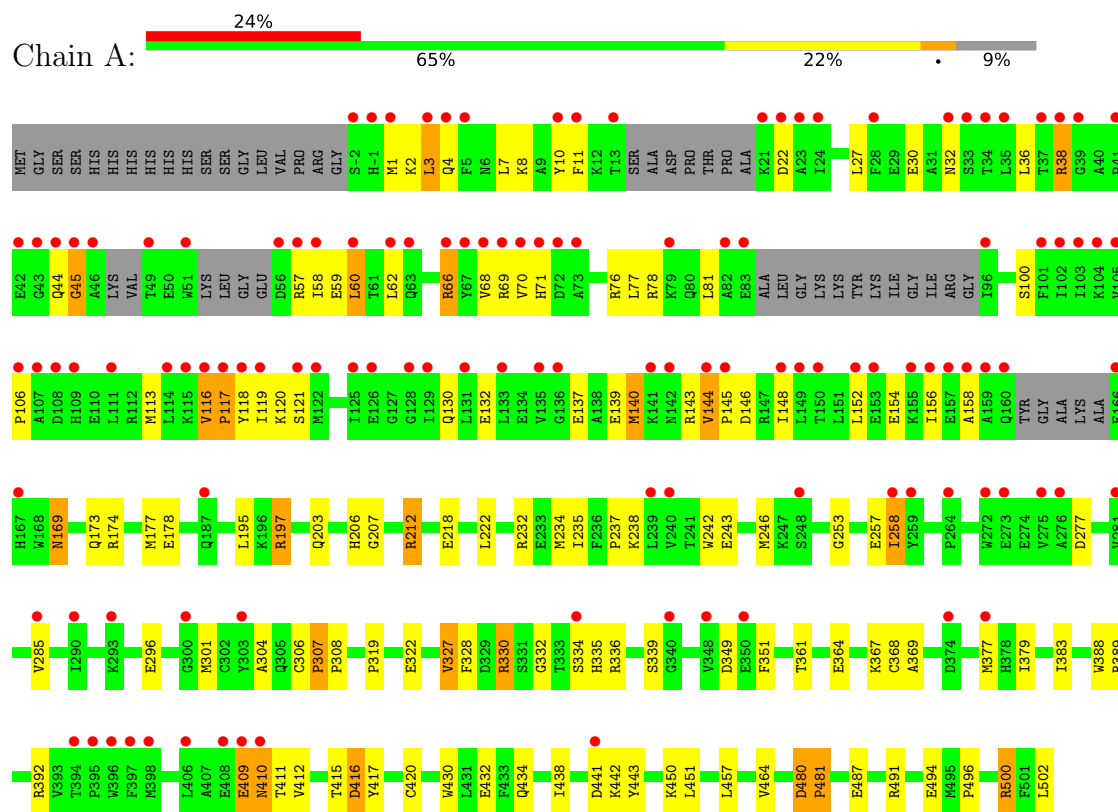
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total 57	O 57	0	0
5	B	42	Total 42	O 42	0	0

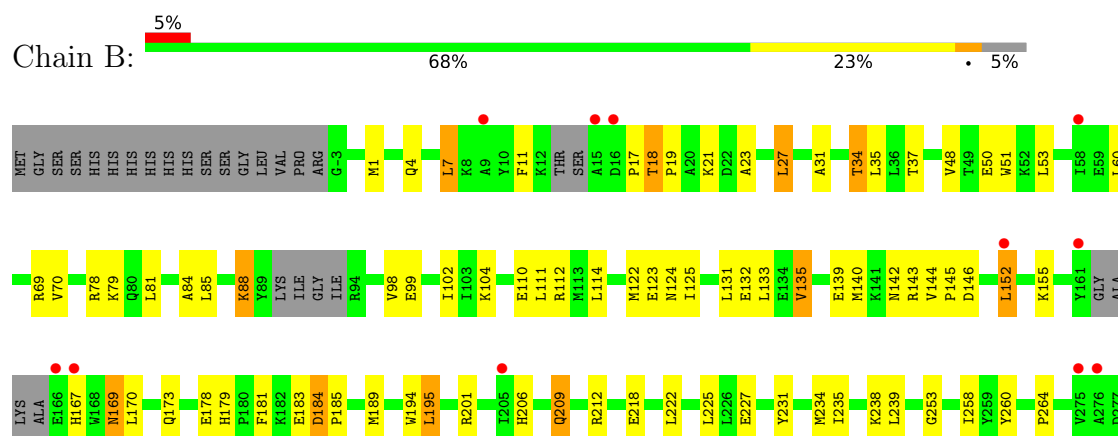
3 Residue-property plots

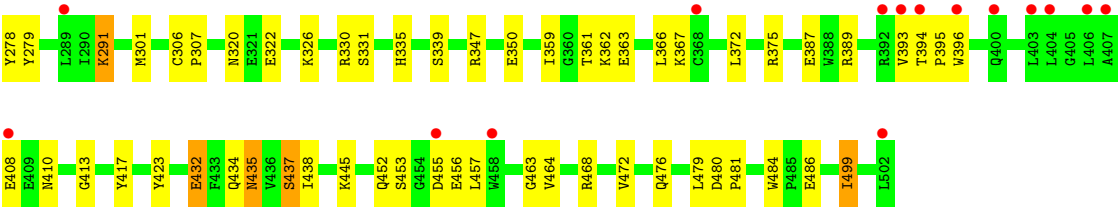
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SERYL-TRNA SYNTHETASE



• Molecule 1: SERYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.93Å 96.93Å 270.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.70 19.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.94-2.70) 98.4 (19.94-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.272 0.225 , 0.271	Depositor DCC
R_{free} test set	2036 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8045	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.63	1/3988 (0.0%)	0.92	7/5390 (0.1%)
1	B	0.59	0/4150	0.88	4/5610 (0.1%)
All	All	0.61	1/8138 (0.0%)	0.90	11/11000 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	VAL	CA-CB	6.16	1.58	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	ASP	CA-C-N	7.20	127.82	119.47
1	B	480	ASP	C-N-CA	7.20	127.82	119.47
1	A	480	ASP	CA-C-N	6.96	128.53	119.84
1	A	480	ASP	C-N-CA	6.96	128.53	119.84
1	A	332	GLY	N-CA-C	6.65	119.10	110.45
1	A	144	VAL	N-CA-CB	6.37	114.51	110.50
1	B	184	ASP	CA-C-N	6.15	126.05	119.28
1	B	184	ASP	C-N-CA	6.15	126.05	119.28
1	A	116	VAL	CA-C-N	5.62	126.86	119.84
1	A	116	VAL	C-N-CA	5.62	126.86	119.84
1	A	57	ARG	N-CA-C	5.37	116.19	107.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3886	0	3795	90	0
1	B	4042	0	3962	86	0
2	A	7	0	4	1	0
2	B	7	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	57	0	0	4	0
5	B	42	0	0	3	0
All	All	8045	0	7765	162	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 10.

All (162) 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:1:MET:HG2	1:A:2:LYS:H	1.27	1.00
1:A:500:ARG:HH11	1:A:500:ARG:HG3	1.22	0.98
1:A:330:ARG:HH11	1:A:330:ARG:HG3	1.27	0.96
1:A:417:TYR:HB2	1:A:434:GLN:HB3	1.54	0.90
1:A:197:ARG:HD2	5:A:2038:HOH:O	1.73	0.89
1:A:1:MET:HG2	1:A:2:LYS:N	1.96	0.81
1:B:225:LEU:HD21	1:B:372:LEU:CD2	2.14	0.77
1:B:110:GLU:HG3	1:B:124:ASN:HD21	1.47	0.77
1:B:417:TYR:HB2	1:B:434:GLN:HB3	1.67	0.77
1:A:139:GLU:O	1:A:144:VAL:HG22	1.88	0.74
1:A:500:ARG:HG3	1:A:500:ARG:NH1	2.01	0.73
1:B:98:VAL:HG21	1:B:140:MET:HE3	1.71	0.73
1:B:339:SER:HB3	5:B:2030:HOH:O	1.87	0.73
1:B:189:MET:HE3	1:B:194:TRP:HE3	1.53	0.72
1:A:434:GLN:HE22	1:A:464:VAL:HG22	1.55	0.71
1:B:366:LEU:HD22	1:B:438:ILE:HD13	1.72	0.71
1:A:301[A]:MET:HE3	1:B:301[A]:MET:HG2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HH11	1:A:330:ARG:CG	2.01	0.70
1:B:209:GLN:HE21	1:B:209:GLN:H	1.39	0.69
1:A:197:ARG:HH12	1:A:203:GLN:H	1.37	0.69
1:A:369:ALA:HB2	1:A:438:ILE:HD11	1.73	0.69
1:A:502:LEU:HD11	1:B:452:GLN:HG3	1.76	0.68
1:A:3:LEU:HD22	1:A:66:ARG:HB2	1.75	0.67
1:A:410:ASN:H	1:A:410:ASN:HD22	1.41	0.66
1:A:10:TYR:HB2	1:A:58:ILE:O	1.97	0.65
1:A:235:ILE:HB	1:B:206:HIS:HB2	1.78	0.64
1:A:306:CYS:SG	1:A:307:PRO:HD3	2.38	0.63
1:B:18:THR:HB	1:B:19:PRO:HD3	1.80	0.62
1:A:173:GLN:HG3	1:A:389:ARG:HB3	1.82	0.62
1:B:181:PHE:CZ	1:B:183:GLU:HG3	2.35	0.61
1:A:409:GLU:HG2	1:A:412:VAL:HG23	1.82	0.60
1:B:396:TRP:CD1	1:B:437:SER:HG	2.19	0.60
1:B:167:HIS:HB3	5:B:2009:HOH:O	2.01	0.59
1:A:246:MET:HG2	1:B:279:TYR:HE1	1.68	0.59
1:A:7:LEU:CB	1:A:70:VAL:HG11	2.32	0.59
1:B:144:VAL:CG1	1:B:145:PRO:HD3	2.33	0.59
1:A:451:LEU:HB2	1:A:457:LEU:HD21	1.83	0.58
1:A:7:LEU:HB3	1:A:70:VAL:HG11	1.86	0.58
1:A:11:PHE:HE1	1:A:78:ARG:HD2	1.69	0.58
1:B:173:GLN:HG3	1:B:389:ARG:HB3	1.86	0.58
1:A:60:LEU:HD13	1:A:77:LEU:HD13	1.86	0.57
1:A:116:VAL:HB	1:A:119:ILE:HD12	1.85	0.57
1:A:143:ARG:O	1:A:146:ASP:HB2	2.06	0.56
1:A:417:TYR:CB	1:A:434:GLN:HB3	2.33	0.56
1:B:225:LEU:HD21	1:B:372:LEU:HD23	1.86	0.56
1:A:361:THR:OG1	1:A:364:GLU:HG3	2.05	0.55
1:B:393:VAL:CG1	1:B:394:THR:N	2.69	0.55
1:B:69:ARG:NH1	1:B:146:ASP:OD2	2.40	0.55
1:A:212:ARG:CZ	1:A:496:PRO:HD3	2.37	0.54
1:A:246:MET:HG2	1:B:279:TYR:CE1	2.42	0.54
1:B:231:TYR:CZ	1:B:326:LYS:HD2	2.43	0.54
1:A:118:TYR:HB2	1:A:148:ILE:HD11	1.90	0.53
1:A:328:PHE:HE2	1:A:330:ARG:HD3	1.74	0.53
1:B:139:GLU:HB3	1:B:144:VAL:CG1	2.38	0.52
1:B:110:GLU:HG3	1:B:124:ASN:ND2	2.22	0.52
1:B:306:CYS:SG	1:B:307:PRO:HD3	2.49	0.52
1:A:206:HIS:HB2	1:B:235:ILE:HB	1.92	0.52
1:A:237:PRO:HD2	1:A:308:PRO:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HG12	1:B:145:PRO:HD3	1.92	0.52
1:B:238:LYS:NZ	1:B:331:SER:OG	2.42	0.52
1:A:8:LYS:HB2	1:A:100:SER:HB3	1.93	0.51
1:A:69:ARG:HA	5:A:2004:HOH:O	2.09	0.51
1:A:174:ARG:NH2	1:A:177:MET:SD	2.84	0.51
1:B:131:LEU:HD11	1:B:152:LEU:HD22	1.91	0.51
1:A:36:LEU:HD23	1:A:76:ARG:HD2	1.93	0.51
1:B:320:ASN:HD21	1:B:453:SER:H	1.57	0.51
1:A:144:VAL:HG23	1:A:145:PRO:HD3	1.93	0.50
1:A:121:SER:HB2	1:A:132:GLU:HB3	1.94	0.50
1:B:225:LEU:HD21	1:B:372:LEU:HD22	1.92	0.50
1:A:330:ARG:CG	1:A:330:ARG:NH1	2.67	0.49
1:B:238:LYS:HB3	1:B:301[B]:MET:HE1	1.94	0.49
1:B:481:PRO:HA	1:B:484:TRP:CD2	2.48	0.48
1:A:379:ILE:HA	1:A:383:ILE:HD13	1.95	0.48
1:A:197:ARG:NH1	1:A:203:GLN:O	2.47	0.48
1:B:11:PHE:HE1	1:B:78:ARG:HB2	1.79	0.48
1:B:445:LYS:NZ	1:B:456:GLU:OE1	2.38	0.48
1:A:243:GLU:HA	1:A:246:MET:HE3	1.95	0.48
1:A:410:ASN:H	1:A:410:ASN:ND2	2.10	0.48
1:A:207:GLY:HA2	1:B:234:MET:HE3	1.96	0.47
1:A:301[A]:MET:HG2	1:B:301[A]:MET:HE3	1.95	0.47
1:B:189:MET:HE2	1:B:195:LEU:HG	1.96	0.47
1:A:500:ARG:HB2	1:B:322:GLU:OE1	2.15	0.47
1:A:197:ARG:CD	5:A:2038:HOH:O	2.48	0.47
1:A:7:LEU:HB2	1:A:70:VAL:HG11	1.97	0.47
1:B:306:CYS:O	1:B:307:PRO:C	2.56	0.46
1:A:238:LYS:N	1:B:350:GLU:OE2	2.45	0.46
1:A:442:LYS:NZ	5:A:2050:HOH:O	2.48	0.46
1:B:435:ASN:C	1:B:435:ASN:HD22	2.24	0.46
1:A:336:ARG:HG3	1:A:351:PHE:HE2	1.80	0.46
1:B:23:ALA:O	1:B:27:LEU:HB2	2.16	0.46
1:B:112:ARG:HH11	1:B:114:LEU:HD11	1.81	0.46
1:B:179:HIS:NE2	1:B:387:GLU:OE1	2.49	0.46
1:B:84:ALA:O	1:B:88:LYS:HB3	2.15	0.46
1:A:307:PRO:HB2	1:A:308:PRO:HD3	1.98	0.46
1:A:234:MET:SD	1:A:327:VAL:HG21	2.56	0.45
1:B:472:VAL:O	1:B:476:GLN:HG3	2.17	0.45
1:A:117:PRO:HG3	1:B:278:TYR:HA	1.98	0.45
1:A:296:GLU:HA	1:B:291:LYS:HG3	1.98	0.45
1:B:434:GLN:HE22	1:B:464:VAL:HG22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:O	1:B:264:PRO:HD3	2.16	0.45
1:A:144:VAL:CG2	1:A:145:PRO:HD3	2.47	0.45
1:B:366:LEU:CD2	1:B:438:ILE:HD13	2.45	0.45
1:A:169:ASN:HD21	1:A:392:ARG:HB3	1.82	0.44
1:B:139:GLU:HB3	1:B:144:VAL:HG11	1.99	0.44
1:B:185:PRO:O	1:B:189:MET:HG3	2.17	0.44
1:A:500:ARG:NH1	1:A:500:ARG:CG	2.72	0.44
1:B:306:CYS:N	1:B:307:PRO:CD	2.80	0.44
1:B:435:ASN:ND2	1:B:463:GLY:H	2.15	0.44
1:A:2:LYS:O	1:A:106:PRO:HG3	2.18	0.44
1:B:218:GLU:OE1	1:B:330:ARG:HD2	2.18	0.44
1:B:123:GLU:OE2	1:B:123:GLU:N	2.50	0.44
1:B:359:ILE:HG22	1:B:457:LEU:HD22	1.99	0.44
1:A:442:LYS:HD3	1:A:443:TYR:CE1	2.53	0.44
1:B:231:TYR:CE2	1:B:326:LYS:HB3	2.53	0.44
1:B:361:THR:O	1:B:362:LYS:C	2.61	0.43
1:B:393:VAL:HG12	1:B:394:THR:N	2.33	0.43
1:A:119:ILE:HG22	1:A:120:LYS:N	2.33	0.43
1:A:420:CYS:HB3	1:A:430:TRP:CE2	2.53	0.43
1:A:27:LEU:HA	1:A:30:GLU:HB2	2.01	0.43
1:A:480:ASP:HA	1:A:481:PRO:HD2	1.63	0.43
1:B:7:LEU:HD12	1:B:70:VAL:HB	2.00	0.43
1:A:335:HIS:HA	1:A:349:ASP:O	2.18	0.43
1:A:71:HIS:HB3	1:A:140:MET:HE3	1.99	0.43
1:B:222:LEU:O	1:B:227:GLU:HG3	2.18	0.43
1:A:58:ILE:HG22	1:A:59:GLU:H	1.84	0.43
1:B:144:VAL:HG13	1:B:145:PRO:HD3	1.99	0.43
1:B:258:ILE:HD11	1:B:260:TYR:CE2	2.53	0.43
1:A:197:ARG:CZ	1:A:197:ARG:HB3	2.49	0.43
1:A:487:GLU:OE1	1:A:491:ARG:NH1	2.52	0.43
1:B:34:THR:O	1:B:37:THR:HB	2.19	0.42
1:A:119:ILE:CG2	1:A:120:LYS:N	2.83	0.42
1:B:169:ASN:O	1:B:169:ASN:ND2	2.53	0.42
1:B:184:ASP:HA	1:B:185:PRO:HD2	1.88	0.42
1:A:368:CYS:O	1:A:369:ALA:C	2.63	0.42
1:B:114:LEU:N	5:B:2005:HOH:O	2.53	0.42
1:A:11:PHE:CE1	1:A:78:ARG:HD2	2.52	0.42
1:A:71:HIS:HB2	1:A:140:MET:HB2	2.00	0.42
1:B:142:ASN:O	1:B:143:ARG:HB2	2.20	0.42
1:A:242:TRP:O	1:A:243:GLU:C	2.61	0.41
1:B:395:PRO:HG3	1:B:413:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:N	1:B:499:ILE:CD1	2.83	0.41
1:A:1:MET:HE2	1:A:1:MET:HB3	1.98	0.41
1:A:416:ASP:OD2	1:A:432:GLU:OE2	2.38	0.41
1:A:441:ASP:OD1	1:A:441:ASP:C	2.64	0.41
1:B:1:MET:HE1	1:B:125:ILE:CD1	2.51	0.41
1:B:432:GLU:O	1:B:468:ARG:HD2	2.20	0.41
1:A:277:ASP:OD2	1:B:155:LYS:NZ	2.37	0.41
1:A:334:SER:C	1:A:335:HIS:CD2	2.99	0.41
1:B:98:VAL:CG2	1:B:140:MET:HE3	2.46	0.41
1:B:31:ALA:HA	1:B:35:LEU:HB3	2.01	0.41
1:A:319:PRO:HD2	1:A:322:GLU:HG3	2.03	0.41
1:B:184:ASP:HB2	1:B:423:TYR:CD1	2.55	0.41
1:B:335:HIS:CE1	1:B:350:GLU:HG3	2.55	0.41
1:A:304:ALA:O	2:A:1505:SER:N	2.54	0.41
1:B:4:GLN:CG	1:B:104:LYS:HB2	2.51	0.41
1:B:170:LEU:HD21	1:B:389:ARG:HD2	2.02	0.41
1:B:135:VAL:HG13	1:B:139:GLU:HB2	2.03	0.41
1:B:231:TYR:CD2	1:B:326:LYS:HB3	2.56	0.40
1:B:499:ILE:N	1:B:499:ILE:HD12	2.36	0.40
1:A:156:ILE:C	1:A:158:ALA:H	2.29	0.40
1:A:44:GLN:O	1:A:45:GLY:C	2.63	0.40
1:A:377:MET:HG3	1:A:388:TRP:CZ2	2.56	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	463/522 (89%)	421 (91%)	35 (8%)	7 (2%)	8	22
1	B	488/522 (94%)	452 (93%)	33 (7%)	3 (1%)	21	44
All	All	951/1044 (91%)	873 (92%)	68 (7%)	10 (1%)	11	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLY
1	A	38	ARG
1	A	4	GLN
1	A	253	GLY
1	B	18	THR
1	B	253	GLY
1	A	68	VAL
1	B	17	PRO
1	A	481	PRO
1	A	117	PRO

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	410/444 (92%)	372 (91%)	38 (9%)	8	21
1	B	424/444 (96%)	382 (90%)	42 (10%)	7	19
All	All	834/888 (94%)	754 (90%)	80 (10%)	8	20

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	22	ASP
1	A	32	ASN
1	A	38	ARG
1	A	60	LEU
1	A	62	LEU
1	A	66	ARG
1	A	81	LEU
1	A	113	MET
1	A	130	GLN
1	A	137	GLU
1	A	140	MET
1	A	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	GLU
1	A	169	ASN
1	A	178	GLU
1	A	195	LEU
1	A	197	ARG
1	A	212	ARG
1	A	218	GLU
1	A	222	LEU
1	A	232	ARG
1	A	257	GLU
1	A	258	ILE
1	A	285	VAL
1	A	307	PRO
1	A	327	VAL
1	A	330	ARG
1	A	339	SER
1	A	367	LYS
1	A	409	GLU
1	A	410	ASN
1	A	411	THR
1	A	415	THR
1	A	416	ASP
1	A	450	LYS
1	A	494	GLU
1	A	500	ARG
1	B	7	LEU
1	B	21	LYS
1	B	27	LEU
1	B	34	THR
1	B	48	VAL
1	B	50	GLU
1	B	51	TRP
1	B	53	LEU
1	B	60	LEU
1	B	79	LYS
1	B	81	LEU
1	B	85	LEU
1	B	88	LYS
1	B	99	GLU
1	B	102	ILE
1	B	111	LEU
1	B	122	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	GLU
1	B	133	LEU
1	B	135	VAL
1	B	152	LEU
1	B	169	ASN
1	B	178	GLU
1	B	195	LEU
1	B	201	ARG
1	B	209	GLN
1	B	212	ARG
1	B	239	LEU
1	B	291	LYS
1	B	347	ARG
1	B	363	GLU
1	B	367	LYS
1	B	375	ARG
1	B	408	GLU
1	B	410	ASN
1	B	432	GLU
1	B	435	ASN
1	B	437	SER
1	B	455	ASP
1	B	479	LEU
1	B	486	GLU
1	B	499	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	80	GLN
1	A	130	GLN
1	A	173	GLN
1	A	283	HIS
1	A	320	ASN
1	A	410	ASN
1	A	490	ASN
1	B	124	ASN
1	B	160	GLN
1	B	169	ASN
1	B	209	GLN
1	B	320	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	343	HIS
1	B	410	ASN
1	B	435	ASN
1	B	490	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	SER	B	1505	3	4,6,6	1.10	1 (25%)	2,7,7	1.50	1 (50%)
2	SER	A	1505	3	4,6,6	1.13	1 (25%)	2,7,7	1.71	1 (50%)

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	SER	B	1505	3	-	0/6/6/6	-
2	SER	A	1505	3	-	0/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1505	SER	OXT-C	-2.07	1.24	1.30
2	B	1505	SER	OXT-C	-2.01	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1505	SER	OXT-C-O	-2.36	118.72	124.08
2	B	1505	SER	OXT-C-O	-2.11	119.29	124.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1505	SER	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	474/522 (90%)	1.41	123 (25%) 1 1	47, 96, 152, 163	1 (0%)
1	B	495/522 (94%)	0.70	26 (5%) 32 28	47, 96, 110, 138	1 (0%)
All	All	969/1044 (92%)	1.05	149 (15%) 5 4	47, 96, 143, 163	2 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ALA	9.4
1	A	66	ARG	7.3
1	A	108	ASP	6.3
1	A	158	ALA	5.9
1	A	68	VAL	5.9
1	A	156	ILE	5.8
1	A	105	VAL	5.2
1	A	126	GLU	5.1
1	A	408	GLU	4.9
1	A	160	GLN	4.7
1	A	22	ASP	4.6
1	A	82	ALA	4.5
1	A	131	LEU	4.5
1	A	46	ALA	4.4
1	A	-2	SER	4.4
1	A	106	PRO	4.4
1	B	167	HIS	4.3
1	A	395	PRO	4.3
1	A	129	ILE	4.3
1	A	-1	HIS	4.2
1	A	109	HIS	4.1
1	A	103	ILE	4.1
1	A	149	LEU	4.1
1	B	9	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	396	TRP	3.9
1	A	67	TYR	3.8
1	A	135	VAL	3.7
1	B	407	ALA	3.6
1	A	114	LEU	3.5
1	A	32	ASN	3.5
1	A	39	GLY	3.4
1	A	41	PRO	3.4
1	A	42	GLU	3.4
1	A	23	ALA	3.4
1	B	15	ALA	3.4
1	A	152	LEU	3.3
1	A	398	MET	3.3
1	A	13	THR	3.2
1	A	28	PHE	3.2
1	A	3	LEU	3.2
1	A	116	VAL	3.2
1	B	275	VAL	3.1
1	A	58	ILE	3.1
1	A	11	PHE	3.1
1	A	281	VAL	3.1
1	A	410	ASN	3.0
1	B	161	TYR	3.0
1	A	34	THR	3.0
1	A	276	ALA	3.0
1	A	71	HIS	3.0
1	A	133	LEU	3.0
1	A	43	GLY	3.0
1	A	275	VAL	3.0
1	A	51	TRP	2.9
1	A	441	ASP	2.9
1	A	159	ALA	2.9
1	A	5	PHE	2.9
1	A	240	VAL	2.9
1	A	167	HIS	2.9
1	A	406	LEU	2.8
1	B	406	LEU	2.8
1	A	157	GLU	2.8
1	A	166	GLU	2.8
1	A	73	ALA	2.7
1	A	239	LEU	2.7
1	A	272	TRP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	409	GLU	2.7
1	A	101	PHE	2.7
1	B	394	THR	2.7
1	A	96	ILE	2.7
1	A	144	VAL	2.7
1	B	393	VAL	2.7
1	A	10	TYR	2.6
1	A	300	GLY	2.6
1	A	340	GLY	2.6
1	A	303	TYR	2.6
1	A	45	GLY	2.6
1	A	273	GLU	2.6
1	A	56	ASP	2.6
1	A	35	LEU	2.6
1	A	111	LEU	2.6
1	A	49	THR	2.5
1	B	396	TRP	2.5
1	A	102	ILE	2.5
1	B	152	LEU	2.5
1	A	63	GLN	2.5
1	A	122	MET	2.5
1	A	24	ILE	2.5
1	A	79	LYS	2.5
1	A	125	ILE	2.5
1	A	141	LYS	2.5
1	A	334	SER	2.5
1	B	455	ASP	2.5
1	B	166	GLU	2.5
1	B	404	LEU	2.4
1	A	128	GLY	2.4
1	A	72	ASP	2.4
1	A	374	ASP	2.4
1	A	104	LYS	2.4
1	B	392	ARG	2.4
1	B	58	ILE	2.4
1	A	33	SER	2.4
1	A	38	ARG	2.4
1	A	115	LYS	2.3
1	A	121	SER	2.3
1	A	44	GLN	2.3
1	B	400	GLN	2.3
1	A	148	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118	TYR	2.3
1	A	259	TYR	2.3
1	B	408	GLU	2.3
1	A	136	GLY	2.3
1	B	276	ALA	2.3
1	A	21	LYS	2.3
1	A	83	GLU	2.3
1	A	60	LEU	2.3
1	A	285	VAL	2.3
1	A	397	PHE	2.3
1	A	119	ILE	2.2
1	A	1	MET	2.2
1	A	153	GLU	2.2
1	B	368	CYS	2.2
1	A	117	PRO	2.2
1	A	4	GLN	2.2
1	A	348	VAL	2.2
1	A	145	PRO	2.2
1	B	16	ASP	2.2
1	A	62	LEU	2.1
1	A	187	GLN	2.1
1	B	502	LEU	2.1
1	A	258	ILE	2.1
1	B	458	TRP	2.1
1	A	293	LYS	2.1
1	A	264	PRO	2.1
1	B	403	LEU	2.1
1	A	142	ASN	2.1
1	B	205	ILE	2.1
1	A	350	GLU	2.1
1	A	377	MET	2.1
1	B	289	LEU	2.1
1	A	70	VAL	2.1
1	A	248	SER	2.0
1	A	150	THR	2.0
1	A	290	ILE	2.0
1	A	57	ARG	2.0
1	A	69	ARG	2.0
1	A	155	LYS	2.0
1	A	37	THR	2.0
1	A	394	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 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($\text{\AA}^2$)	Q<0.9
2	SER	A	1505	7/7	0.79	0.23	91,92,93,93	0
2	SER	B	1505	7/7	0.89	0.25	73,74,74,74	0
4	CL	A	1504	1/1	0.96	0.22	56,56,56,56	0
4	CL	B	1504	1/1	0.98	0.23	58,58,58,58	0
3	ZN	A	1503	1/1	0.99	0.20	83,83,83,83	0
3	ZN	B	1503	1/1	0.99	0.18	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.