Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:17 AM GMT

PDB ID	:	2CJB
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
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 (1)) were used in the production of this report:

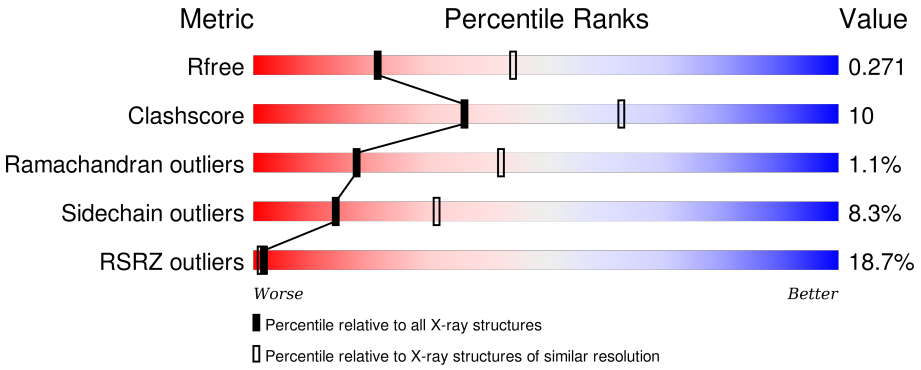
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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.

Mol	Chain	Length	Quality of chain
1	A	522	20% 67% 21% • 9%
1	B	522	15% 71% 22% • 5%

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	SER	A	1505	-	-	-	X
2	SER	B	1505	-	-	-	X

2 Entry composition

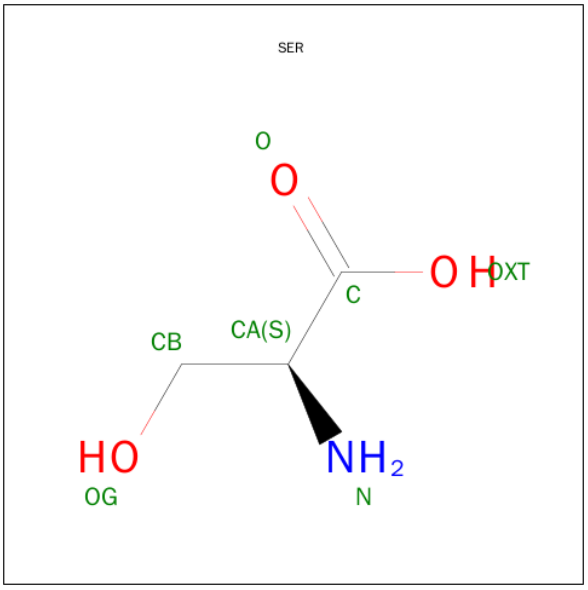
There are 5 unique types of molecules in this entry. The entry contains 8045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 5 is water.

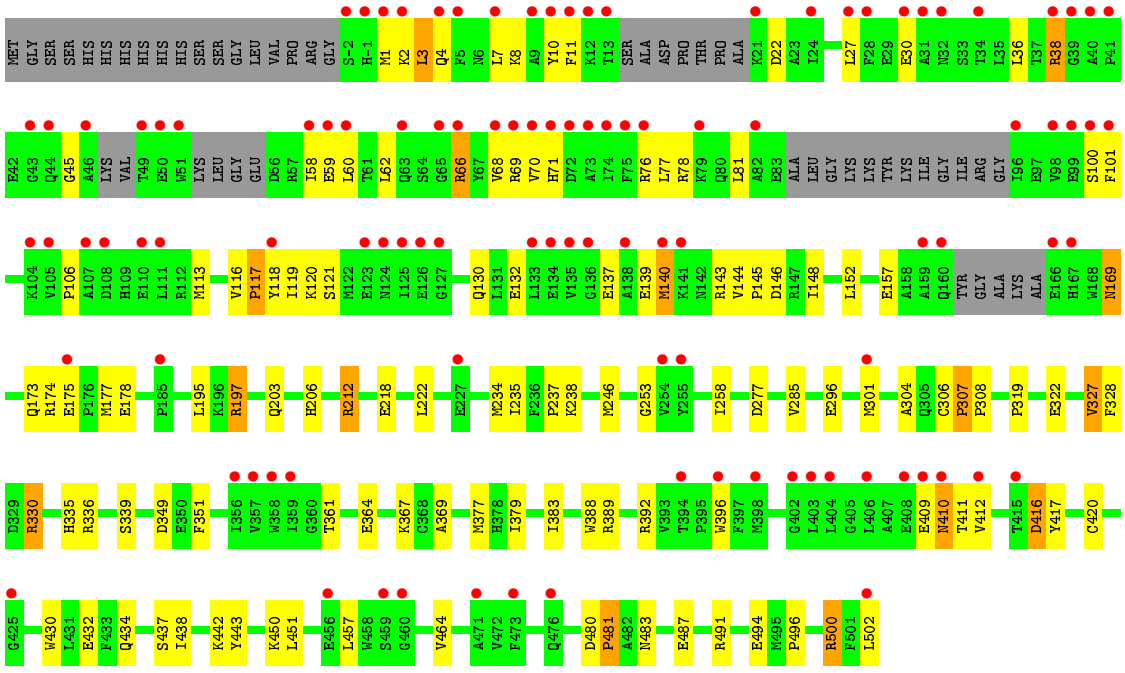
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	57	Total O 57 57	0	0
5	B	42	Total O 42 42	0	0

3 Residue-property plots (i)

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

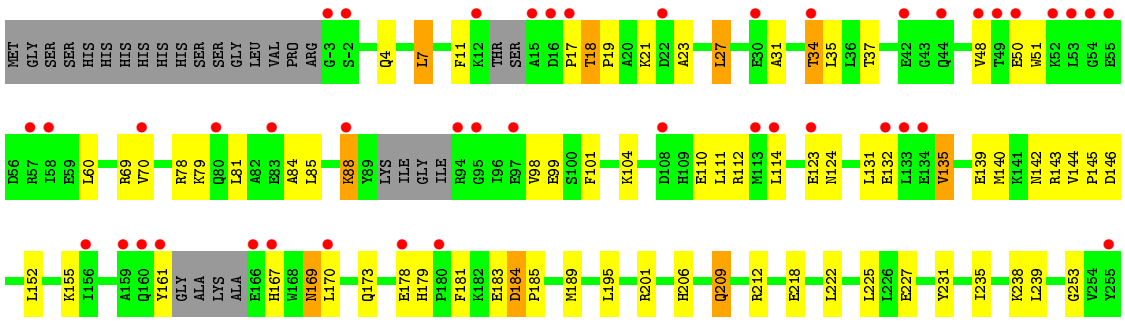
- Molecule 1: SERYL-TRNA SYNTHETASE

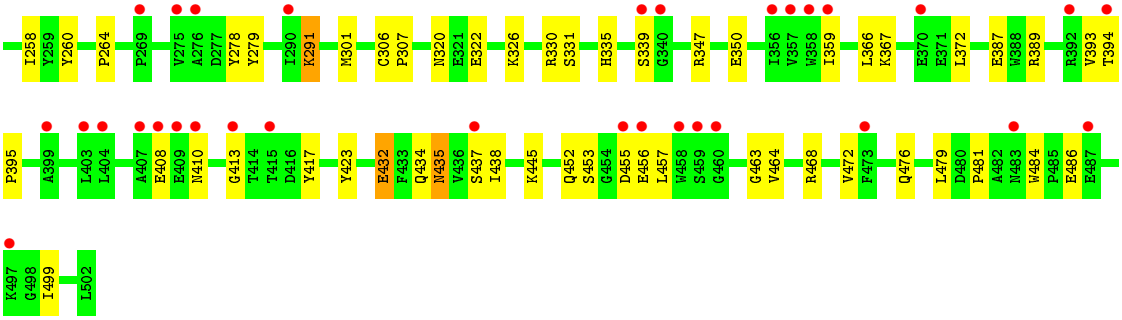
Chain A:



- Molecule 1: SERYL-TRNA SYNTHETASE

Chain B:




I258 Y259 Y260 P264 P269 V275 A276 D277 Y278 Y279 I290 K291 M301 C306 P307 N320 E321 E322 K326 R330 S331 H335 S339 G340 R347 E350 I356 V357 W358 I359 L366 K367 E370 E371 L372 E387 W388 R389 R392 V393 T394
P395 A399 L403 L404 A407 E408 E409 N410 G413 T414 T415 D416 Y417 Y423 E432 F433 Q434 N435 V436 S437 I438 K445 Q452 S453 G454 D455 E456 L457 W458 S459 G460 G463 V464 R468 V472 F473 Q476 L479 D480 P481 A482 N483 W484 P485 E486 E487
K497 G498 I499 L502

4 Data and refinement statistics (i)

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) 98.7 (19.94-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.26%)	DCC
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 , 77.8	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 40777 reflections	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/3988	0.64	0/5390
1	B	0.49	0/4150	0.64	2/5610 (0.0%)
All	All	0.51	0/8138	0.64	2/11000 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	184	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	184	ASP	CB-CG-OD2	-5.15	113.66	118.30

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	82	0
1	B	4042	0	3962	82	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	150	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 (150) 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:NH1	1:A:500:ARG:HG3	2.01	0.73
1:B:339:SER:HB3	5:B:2030:HOH:O	1.87	0.73
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:330:ARG:CG	1:A:330:ARG:HH11	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:301[A]:MET:HG2	1:B:301[A]:MET:HE3	1.82	0.61
1:A:409:GLU:HG2	1:A:412:VAL:HG23	1.82	0.60
1:B:167:HIS:HB3	5:B:2009:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:98:VAL:HG21	1:B:140:MET:HE3	1.86	0.57
1:A:116:VAL:HB	1:A:119:ILE:HD12	1.85	0.57
1:A:417:TYR:CB	1:A:434:GLN:HB3	2.33	0.56
1:A:143:ARG:O	1:A:146:ASP:HB2	2.06	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:B:238:LYS:HB3	1:B:301[B]:MET:HE1	1.91	0.53
1:A:328:PHE:HE2	1:A:330:ARG:HD3	1.74	0.53
1:A:118:TYR:HB2	1:A:148:ILE:HD11	1.90	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:237:PRO:HD2	1:A:308:PRO:HB2	1.92	0.52
1:A:206:HIS:HB2	1:B:235:ILE:HB	1.92	0.52
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:B:131:LEU:HD11	1:B:152:LEU:HD22	1.91	0.51
1:A:174:ARG:NH2	1:A:177:MET:SD	2.84	0.51
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: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:396:TRP:HD1	1:A:437:SER:HG	1.59	0.50
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:481:PRO:HA	1:B:484:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:277:ASP:OD2	1:B:155:LYS:NZ	2.37	0.48
1:A:410:ASN:H	1:A:410:ASN:ND2	2.10	0.48
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:A:442:LYS:NZ	5:A:2050:HOH:O	2.48	0.46
1:A:238:LYS:N	1:B:350:GLU:OE2	2.45	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:179:HIS:NE2	1:B:387:GLU:OE1	2.49	0.46
1:B:112:ARG:HH11	1:B:114:LEU:HD11	1.81	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:B:434:GLN:HE22	1:B:464:VAL:HG22	1.82	0.45
1:A:296:GLU:HA	1:B:291:LYS:HG3	1.98	0.45
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:B:393:VAL:HG12	1:B:394:THR:N	2.33	0.44
1:B:306:CYS:O	1:B:307:PRO:C	2.56	0.44
1:A:2:LYS:O	1:A:106:PRO:HG3	2.18	0.44
1:A:301[A]:MET:HE3	1:B:301[A]:MET:HG2	2.00	0.44
1:B:218:GLU:OE1	1:B:330:ARG:HD2	2.18	0.44
1:B:359:ILE:HG22	1:B:457:LEU:HD22	1.99	0.44
1:B:123:GLU:OE2	1:B:123:GLU:N	2.50	0.44
1:B:231:TYR:CE2	1:B:326:LYS:HB3	2.53	0.44
1:A:442:LYS:HD3	1:A:443:TYR:CE1	2.53	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD12	1:B:70:VAL:HB	2.00	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:A:335:HIS:HA	1:A:349:ASP:O	2.18	0.43
1:B:101:PHE:HD2	1:B:140:MET:HE2	1.84	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:B:101:PHE:CD2	1:B:140:MET:HE2	2.54	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:184:ASP:HA	1:B:185:PRO:HD2	1.88	0.42
1:B:169:ASN:O	1:B:169:ASN:ND2	2.53	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:B:395:PRO:HG3	1:B:413:GLY:HA2	2.02	0.41
1:B:435:ASN:C	1:B:435:ASN:HD22	2.24	0.41
1:B:499:ILE:CD1	1:B:499:ILE:N	2.83	0.41
1:A:416:ASP:OD2	1:A:432:GLU:OE2	2.38	0.41
1:B:432:GLU:O	1:B:468:ARG:HD2	2.20	0.41
1:B:445:LYS:NZ	1:B:456:GLU:OE1	2.38	0.41
1:B:31:ALA:HA	1:B:35:LEU:HB3	2.01	0.41
1:B:335:HIS:CE1	1:B:350:GLU:HG3	2.55	0.41
1:B:184:ASP:HB2	1:B:423:TYR:CD1	2.55	0.41
1:A:319:PRO:HD2	1:A:322:GLU:HG3	2.03	0.41
1:A:301[A]:MET:CE	1:B:301[A]:MET:HG2	2.51	0.41
1:B:170:LEU:HD21	1:B:389:ARG:HD2	2.02	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: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:377:MET:HG3	1:A:388:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/522 (89%)	421 (91%)	35 (8%)	7 (2%)	13	32
1	B	488/522 (94%)	452 (93%)	33 (7%)	3 (1%)	30	59
All	All	951/1044 (91%)	873 (92%)	68 (7%)	10 (1%)	17	42

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%)	376 (92%)	34 (8%)	14	31
1	B	424/444 (96%)	389 (92%)	35 (8%)	14	31
All	All	834/888 (94%)	765 (92%)	69 (8%)	14	31

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	22	ASP
1	A	38	ARG
1	A	62	LEU
1	A	66	ARG
1	A	81	LEU
1	A	101	PHE
1	A	113	MET
1	A	130	GLN
1	A	137	GLU
1	A	140	MET
1	A	152	LEU
1	A	157	GLU
1	A	169	ASN
1	A	175	GLU
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	285	VAL
1	A	307	PRO
1	A	327	VAL
1	A	330	ARG
1	A	339	SER
1	A	367	LYS
1	A	410	ASN
1	A	411	THR
1	A	416	ASP
1	A	450	LYS
1	A	483	ASN
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	60	LEU

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Mol	Chain	Res	Type
1	B	79	LYS
1	B	81	LEU
1	B	85	LEU
1	B	88	LYS
1	B	99	GLU
1	B	111	LEU
1	B	132	GLU
1	B	135	VAL
1	B	161	TYR
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	367	LYS
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

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

Mol	Chain	Res	Type
1	A	80	GLN
1	A	130	GLN
1	A	169	ASN
1	A	283	HIS
1	A	410	ASN
1	A	434	GLN
1	A	490	ASN
1	B	6	ASN
1	B	109	HIS
1	B	124	ASN
1	B	160	GLN

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Mol	Chain	Res	Type
1	B	169	ASN
1	B	209	GLN
1	B	320	ASN
1	B	343	HIS
1	B	410	ASN
1	B	435	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

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	A	1505	3	3,6,6	0.47	0	1,7,7	0.28	0
2	SER	B	1505	3	3,6,6	0.48	0	1,7,7	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SER	A	1505	3	-	0/2/6/6	0/0/0/0
2	SER	B	1505	3	-	0/2/6/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	1.23	105 (22%) 1 1	85, 96, 152, 163	0
1	B	495/522 (94%)	0.87	76 (15%) 3 2	81, 96, 110, 138	0
All	All	969/1044 (92%)	1.05	181 (18%) 2 1	81, 96, 143, 163	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	PHE	13.2
1	A	-2	SER	11.4
1	A	43	GLY	8.2
1	A	71	HIS	8.0
1	A	28	PHE	7.9
1	B	49	THR	7.6
1	A	46	ALA	7.1
1	B	407	ALA	7.0
1	B	54	GLY	7.0
1	A	10	TYR	7.0
1	A	74	ILE	6.7
1	A	68	VAL	6.4
1	A	66	ARG	6.4
1	A	60	LEU	5.9
1	A	160	GLN	5.8
1	A	13	THR	5.7
1	A	502	LEU	5.7
1	A	159	ALA	5.7
1	B	408	GLU	5.5
1	B	459	SER	5.4
1	B	167	HIS	5.3
1	A	9	ALA	5.2
1	A	34	THR	5.2
1	B	113	MET	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	409	GLU	5.1
1	A	63	GLN	5.1
1	B	409	GLU	5.0
1	A	408	GLU	4.8
1	A	49	THR	4.8
1	A	98	VAL	4.6
1	B	16	ASP	4.5
1	A	12	LYS	4.4
1	A	58	ILE	4.3
1	B	460	GLY	4.3
1	B	161	TYR	4.2
1	B	94	ARG	4.1
1	A	107	ALA	4.1
1	B	55	GLU	4.1
1	B	159	ALA	4.1
1	A	410	ASN	4.1
1	A	127	GLY	4.1
1	A	69	ARG	4.0
1	B	394	THR	4.0
1	A	7	LEU	4.0
1	A	27	LEU	3.9
1	B	108	ASP	3.9
1	A	459	SER	3.9
1	A	-1	HIS	3.9
1	A	108	ASP	3.8
1	A	39	GLY	3.8
1	B	340	GLY	3.7
1	B	404	LEU	3.7
1	A	403	LEU	3.7
1	A	70	VAL	3.6
1	A	73	ALA	3.6
1	B	359	ILE	3.6
1	A	301[A]	MET	3.6
1	A	460	GLY	3.6
1	A	5	PHE	3.5
1	A	24	ILE	3.5
1	B	12	LYS	3.5
1	A	96	ILE	3.5
1	A	44	GLN	3.4
1	A	59	GLU	3.4
1	A	166	GLU	3.4
1	A	72	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	15	ALA	3.3
1	A	404	LEU	3.3
1	B	413	GLY	3.2
1	B	356	ILE	3.2
1	A	141	LYS	3.2
1	B	-3	GLY	3.2
1	A	111	LEU	3.1
1	A	167	HIS	3.1
1	B	58	ILE	3.1
1	A	135	VAL	3.1
1	B	392	ARG	3.0
1	A	398	MET	3.0
1	A	75	PHE	3.0
1	A	76	ARG	3.0
1	B	160	GLN	3.0
1	B	370	GLU	2.9
1	A	65	GLY	2.9
1	B	180	PRO	2.9
1	A	30	GLU	2.9
1	A	227	GLU	2.9
1	B	166	GLU	2.9
1	A	126	GLU	2.9
1	B	255	TYR	2.9
1	A	185	PRO	2.8
1	A	118	TYR	2.8
1	B	53	LEU	2.8
1	B	83	GLU	2.8
1	B	339	SER	2.8
1	A	101	PHE	2.8
1	B	42	GLU	2.8
1	A	51	TRP	2.8
1	A	123	GLU	2.7
1	A	1	MET	2.7
1	A	359	ILE	2.7
1	A	4	GLN	2.7
1	A	476	GLN	2.7
1	A	133	LEU	2.7
1	A	356	ILE	2.7
1	B	17	PRO	2.7
1	A	358	TRP	2.7
1	A	82	ALA	2.7
1	B	437	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	456	GLU	2.6
1	B	473	PHE	2.6
1	B	34	THR	2.6
1	B	22	ASP	2.6
1	A	2	LYS	2.6
1	A	255	TYR	2.6
1	A	105	VAL	2.6
1	B	44	GLN	2.5
1	A	125	ILE	2.5
1	A	357	VAL	2.5
1	A	396	TRP	2.5
1	B	80	GLN	2.5
1	B	357	VAL	2.5
1	A	38	ARG	2.5
1	A	134	GLU	2.5
1	A	100	SER	2.4
1	B	-2	SER	2.4
1	B	57	ARG	2.4
1	B	132	GLU	2.4
1	A	140	MET	2.4
1	A	394	THR	2.4
1	A	124	ASN	2.4
1	A	41	PRO	2.4
1	A	21	LYS	2.4
1	A	471	ALA	2.3
1	A	99	GLU	2.3
1	A	473	PHE	2.3
1	B	48	VAL	2.3
1	B	275	VAL	2.3
1	B	458	TRP	2.3
1	B	123	GLU	2.3
1	B	399	ALA	2.3
1	A	79	LYS	2.3
1	B	497	LYS	2.3
1	B	97	GLU	2.3
1	B	50	GLU	2.2
1	B	410	ASN	2.2
1	A	402	GLY	2.2
1	A	406	LEU	2.2
1	A	415	THR	2.2
1	B	52	LYS	2.2
1	B	88	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	ASN	2.2
1	A	412	VAL	2.2
1	B	114	LEU	2.2
1	A	104	LYS	2.2
1	B	276	ALA	2.2
1	B	415	THR	2.2
1	B	170	LEU	2.2
1	B	403	LEU	2.2
1	A	50	GLU	2.2
1	A	175	GLU	2.2
1	A	456	GLU	2.2
1	A	136	GLY	2.2
1	B	95	GLY	2.2
1	B	483	ASN	2.1
1	B	178	GLU	2.1
1	B	133	LEU	2.1
1	B	156	ILE	2.1
1	A	425	GLY	2.1
1	B	70	VAL	2.1
1	B	30	GLU	2.1
1	B	290	ILE	2.1
1	A	31	ALA	2.1
1	B	487	GLU	2.1
1	B	358	TRP	2.1
1	A	110	GLU	2.1
1	A	254	VAL	2.0
1	A	138	ALA	2.0
1	B	269	PRO	2.0
1	A	40	ALA	2.0
1	B	134	GLU	2.0
1	B	455	ASP	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SER	A	1505	7/7	0.94	0.51	5.35	91,92,93,93	0
2	SER	B	1505	7/7	0.95	0.40	4.14	73,74,74,74	0
3	ZN	A	1503	1/1	0.95	0.22	-0.35	83,83,83,83	0
3	ZN	B	1503	1/1	0.98	0.18	-0.88	81,81,81,81	0
4	CL	B	1504	1/1	0.98	0.13	-2.03	58,58,58,58	0
4	CL	A	1504	1/1	0.91	0.14	-3.84	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.