Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 AM GMT

PDB ID	:	2ODR
Title	:	Methanococcus Maripaludis Phosphoseryl-tRNA synthetase
Authors	:	Steitz, T.A.; Kamtekar, S.
Deposited on	:	2006-12-26
Resolution	:	3.23 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 ⓘ symbol.

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

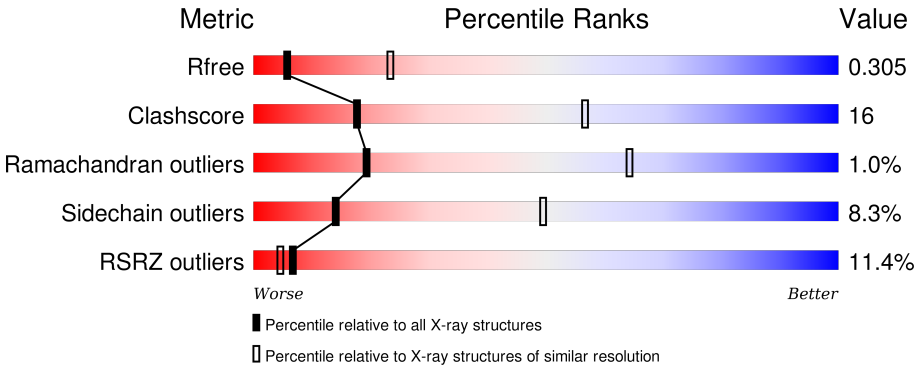
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.23 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	665	5% 54% 17% • 26%
2	B	648	6% 47% 19% • 31%
3	C	701	7% 50% 14% • 33%
4	D	685	5% 50% 14% • 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13538 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 phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3626	2314	613	682	17			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	cloning artifact	UNP Q6LZE1
A	-17	GLY	-	cloning artifact	UNP Q6LZE1
A	-16	SER	-	cloning artifact	UNP Q6LZE1
A	-15	HIS	-	cloning artifact	UNP Q6LZE1
A	-14	HIS	-	cloning artifact	UNP Q6LZE1
A	-13	HIS	-	cloning artifact	UNP Q6LZE1
A	-12	HIS	-	cloning artifact	UNP Q6LZE1
A	-11	HIS	-	cloning artifact	UNP Q6LZE1
A	-10	HIS	-	cloning artifact	UNP Q6LZE1
A	-9	SER	-	cloning artifact	UNP Q6LZE1
A	-8	SER	-	cloning artifact	UNP Q6LZE1
A	-7	GLY	-	cloning artifact	UNP Q6LZE1
A	-6	LEU	-	cloning artifact	UNP Q6LZE1
A	-5	VAL	-	cloning artifact	UNP Q6LZE1
A	-4	PRO	-	cloning artifact	UNP Q6LZE1
A	-3	ARG	-	cloning artifact	UNP Q6LZE1
A	-2	GLY	-	cloning artifact	UNP Q6LZE1
A	-1	SER	-	cloning artifact	UNP Q6LZE1
A	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 2 is a protein called phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	448	Total	C	N	O	S	0	0	0
			3320	2120	559	625	16			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	cloning artifact	UNP Q6LZE1
B	-17	GLY	-	cloning artifact	UNP Q6LZE1
B	-16	SER	-	cloning artifact	UNP Q6LZE1
B	-15	HIS	-	cloning artifact	UNP Q6LZE1
B	-14	HIS	-	cloning artifact	UNP Q6LZE1
B	-13	HIS	-	cloning artifact	UNP Q6LZE1
B	-12	HIS	-	cloning artifact	UNP Q6LZE1
B	-11	HIS	-	cloning artifact	UNP Q6LZE1
B	-10	HIS	-	cloning artifact	UNP Q6LZE1
B	-9	SER	-	cloning artifact	UNP Q6LZE1
B	-8	SER	-	cloning artifact	UNP Q6LZE1
B	-7	GLY	-	cloning artifact	UNP Q6LZE1
B	-6	LEU	-	cloning artifact	UNP Q6LZE1
B	-5	VAL	-	cloning artifact	UNP Q6LZE1
B	-4	PRO	-	cloning artifact	UNP Q6LZE1
B	-3	ARG	-	cloning artifact	UNP Q6LZE1
B	-2	GLY	-	cloning artifact	UNP Q6LZE1
B	-1	SER	-	cloning artifact	UNP Q6LZE1
B	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 3 is a protein called phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	468	Total	C	N	O	S	0	0	0
			3337	2119	577	627	14			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	cloning artifact	UNP Q6LZE1
C	-17	GLY	-	cloning artifact	UNP Q6LZE1
C	-16	SER	-	cloning artifact	UNP Q6LZE1
C	-15	HIS	-	cloning artifact	UNP Q6LZE1
C	-14	HIS	-	cloning artifact	UNP Q6LZE1
C	-13	HIS	-	cloning artifact	UNP Q6LZE1
C	-12	HIS	-	cloning artifact	UNP Q6LZE1
C	-11	HIS	-	cloning artifact	UNP Q6LZE1
C	-10	HIS	-	cloning artifact	UNP Q6LZE1
C	-9	SER	-	cloning artifact	UNP Q6LZE1
C	-8	SER	-	cloning artifact	UNP Q6LZE1
C	-7	GLY	-	cloning artifact	UNP Q6LZE1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	cloning artifact	UNP Q6LZE1
C	-5	VAL	-	cloning artifact	UNP Q6LZE1
C	-4	PRO	-	cloning artifact	UNP Q6LZE1
C	-3	ARG	-	cloning artifact	UNP Q6LZE1
C	-2	GLY	-	cloning artifact	UNP Q6LZE1
C	-1	SER	-	cloning artifact	UNP Q6LZE1
C	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 4 is a protein called phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	451	Total	C	N	O	S	0	0	0
			3255	2071	560	610	14			

There are 19 discrepancies between the modelled and reference sequences:

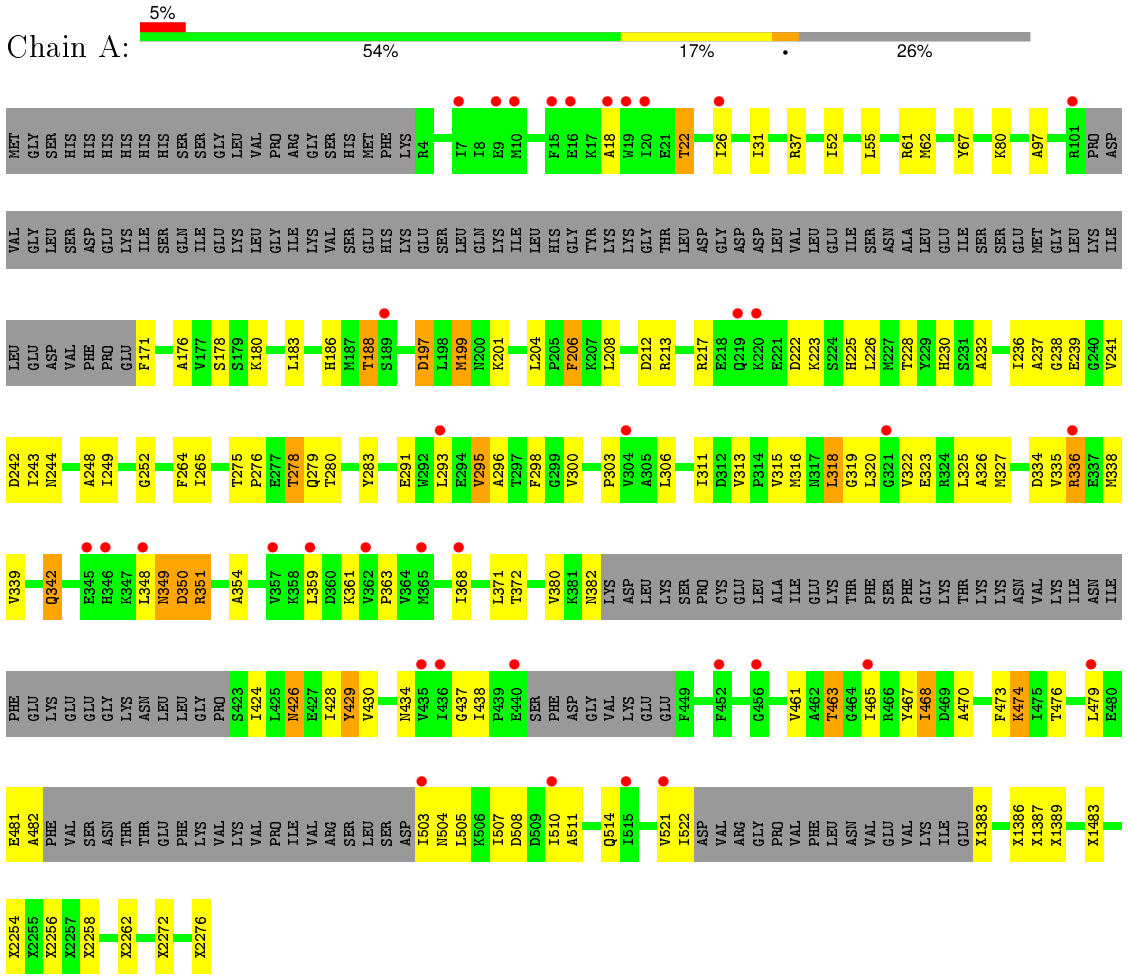
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	cloning artifact	UNP Q6LZE1
D	-17	GLY	-	cloning artifact	UNP Q6LZE1
D	-16	SER	-	cloning artifact	UNP Q6LZE1
D	-15	HIS	-	cloning artifact	UNP Q6LZE1
D	-14	HIS	-	cloning artifact	UNP Q6LZE1
D	-13	HIS	-	cloning artifact	UNP Q6LZE1
D	-12	HIS	-	cloning artifact	UNP Q6LZE1
D	-11	HIS	-	cloning artifact	UNP Q6LZE1
D	-10	HIS	-	cloning artifact	UNP Q6LZE1
D	-9	SER	-	cloning artifact	UNP Q6LZE1
D	-8	SER	-	cloning artifact	UNP Q6LZE1
D	-7	GLY	-	cloning artifact	UNP Q6LZE1
D	-6	LEU	-	cloning artifact	UNP Q6LZE1
D	-5	VAL	-	cloning artifact	UNP Q6LZE1
D	-4	PRO	-	cloning artifact	UNP Q6LZE1
D	-3	ARG	-	cloning artifact	UNP Q6LZE1
D	-2	GLY	-	cloning artifact	UNP Q6LZE1
D	-1	SER	-	cloning artifact	UNP Q6LZE1
D	0	HIS	-	cloning artifact	UNP Q6LZE1

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.

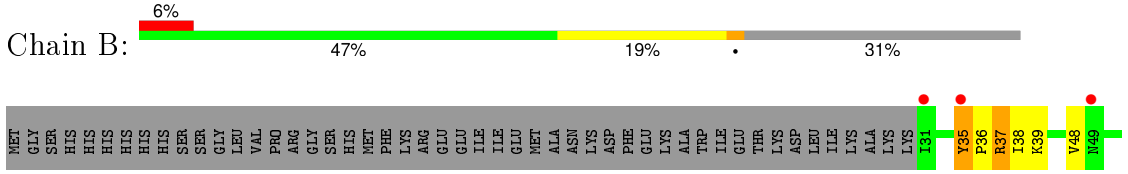
- Molecule 1: phosphoseryl-tRNA synthetase

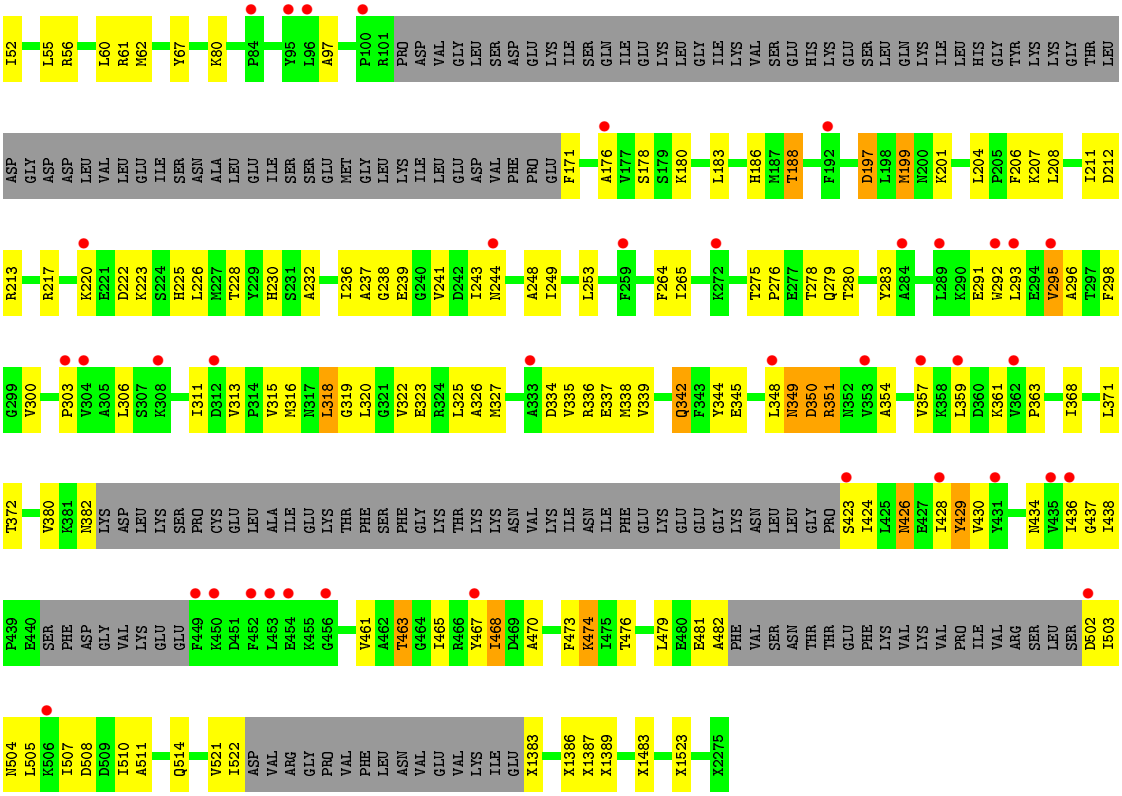
Chain A:



- Molecule 2: phosphoseryl-tRNA synthetase

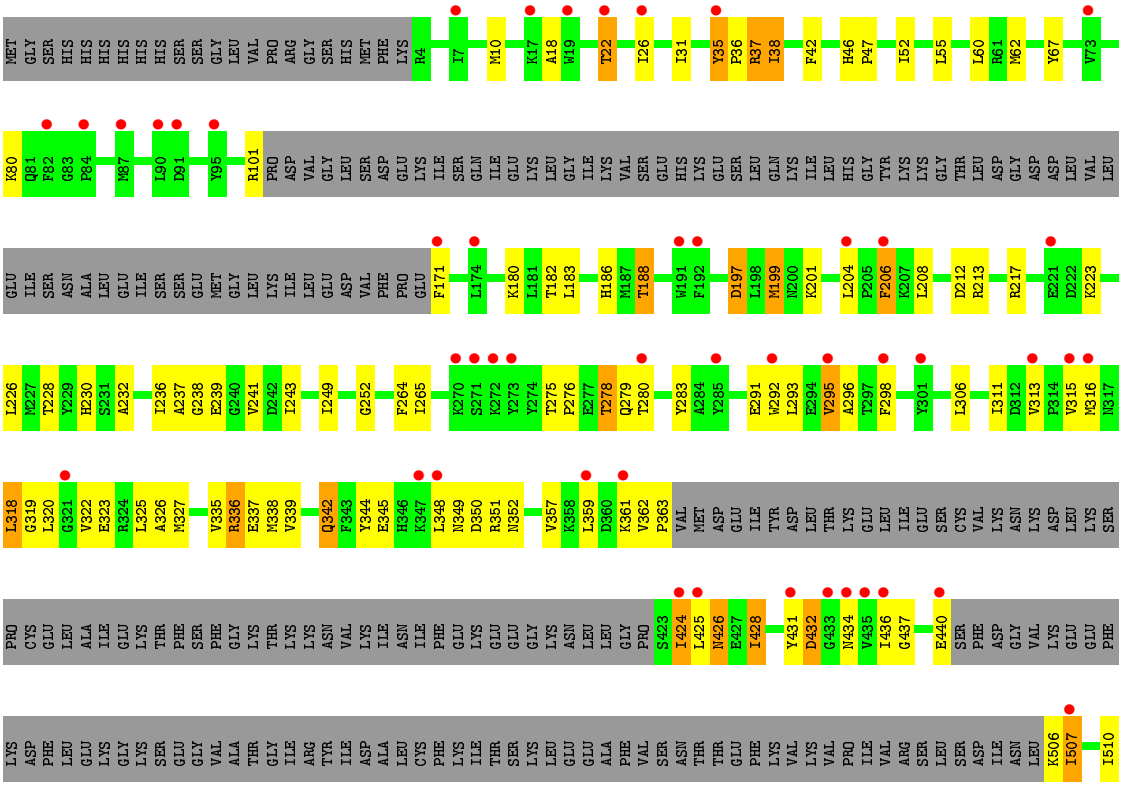
Chain B:

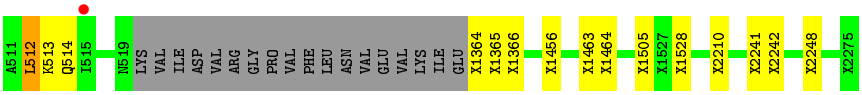




- Molecule 3: phosphoseryl-tRNA synthetase

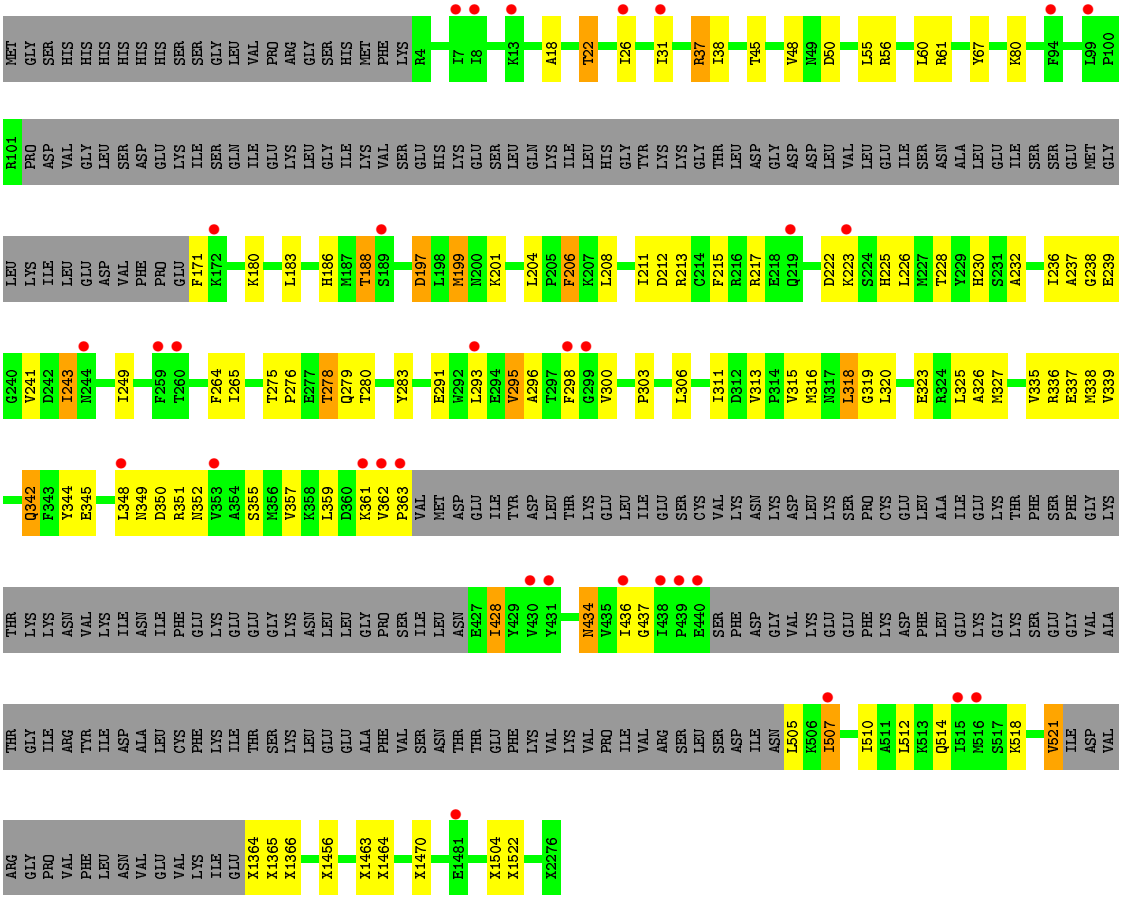
Chain C:





- Molecule 4: phosphoseryl-tRNA synthetase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.17Å 133.94Å 208.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.23 45.23 – 3.23	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.23) 97.9 (45.23-3.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.292 , 0.306 0.292 , 0.305	Depositor DCC
R_{free} test set	2697 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	123.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 163.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 53170 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	0.42	0/3142	0.56	0/4229
2	B	0.43	0/2918	0.57	0/3932
3	C	0.41	0/2669	0.56	0/3597
4	D	0.43	0/2671	0.56	0/3597
All	All	0.42	0/11400	0.56	0/15355

There are no bond length outliers.

There are no bond angle outliers.

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	3626	0	3242	120	0
2	B	3320	0	2990	118	1
3	C	3337	0	2798	93	0
4	D	3255	0	2788	99	1
All	All	13538	0	11818	403	1

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 16.

All (403) 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)
3:C:236:ILE:HD11	3:C:249:ILE:HD11	1.26	1.13
4:D:236:ILE:HD11	4:D:249:ILE:HD11	1.25	1.13
1:A:236:ILE:HD11	1:A:249:ILE:HD11	1.26	1.11
2:B:236:ILE:HD11	2:B:249:ILE:HD11	1.30	1.09
3:C:506:LYS:N	3:C:1505:UNK:C	2.20	1.04
1:A:275:THR:O	1:A:278:THR:HG22	1.58	1.03
3:C:275:THR:O	3:C:278:THR:HG22	1.59	1.02
2:B:275:THR:O	2:B:278:THR:HG22	1.62	1.00
4:D:275:THR:O	4:D:278:THR:HG22	1.61	1.00
4:D:236:ILE:CD1	4:D:249:ILE:HD11	2.00	0.92
3:C:236:ILE:CD1	3:C:249:ILE:HD11	2.01	0.91
1:A:236:ILE:CD1	1:A:249:ILE:HD11	2.01	0.91
1:A:348:LEU:HD11	1:A:510:ILE:HG22	1.54	0.90
4:D:505:LEU:N	4:D:1504:UNK:C	2.34	0.90
4:D:223:LYS:O	4:D:335:VAL:HG22	1.70	0.90
1:A:482:ALA:C	1:A:1483:UNK:N	2.25	0.89
2:B:236:ILE:CD1	2:B:249:ILE:HD11	2.03	0.88
2:B:482:ALA:C	2:B:1483:UNK:N	2.27	0.88
3:C:223:LYS:O	3:C:335:VAL:HG22	1.72	0.87
2:B:223:LYS:O	2:B:335:VAL:HG22	1.72	0.87
2:B:348:LEU:HD11	2:B:510:ILE:HG22	1.58	0.86
1:A:382:ASN:C	1:A:1383:UNK:N	2.28	0.85
1:A:223:LYS:O	1:A:335:VAL:HG22	1.76	0.85
3:C:183:LEU:HD11	4:D:183:LEU:HD11	1.56	0.84
4:D:342:GLN:HE21	4:D:342:GLN:H	1.25	0.82
2:B:382:ASN:C	2:B:1383:UNK:N	2.32	0.82
2:B:342:GLN:HE21	2:B:342:GLN:H	1.27	0.80
1:A:300:VAL:HG11	4:D:26:ILE:HD13	1.65	0.78
1:A:342:GLN:HE21	1:A:342:GLN:H	1.29	0.78
1:A:176:ALA:HB3	2:B:178:SER:OG	1.84	0.77
3:C:342:GLN:HE21	3:C:342:GLN:H	1.31	0.76
3:C:326:ALA:HB3	3:C:338:MET:HE1	1.66	0.74
4:D:199:MET:HE3	4:D:199:MET:HA	1.67	0.74
2:B:368:ILE:O	2:B:476:THR:CG2	2.35	0.74
2:B:368:ILE:O	2:B:476:THR:HG21	1.87	0.74
2:B:326:ALA:HB3	2:B:338:MET:HE1	1.68	0.74
4:D:326:ALA:HB3	4:D:338:MET:HE1	1.70	0.74
1:A:31:ILE:HG21	1:A:359:LEU:HD12	1.67	0.73
4:D:521:VAL:C	4:D:1522:UNK:N	2.42	0.73
1:A:31:ILE:CG2	1:A:359:LEU:HD12	2.18	0.73
1:A:178:SER:OG	2:B:176:ALA:HB3	1.89	0.73
1:A:326:ALA:HB3	1:A:338:MET:HE1	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:337:GLU:HG2	3:C:344:TYR:CD2	2.25	0.71
2:B:199:MET:HE3	2:B:199:MET:HA	1.73	0.71
1:A:368:ILE:O	1:A:476:THR:CG2	2.38	0.71
4:D:199:MET:CE	4:D:199:MET:HA	2.21	0.70
1:A:327:MET:SD	1:A:335:VAL:HG13	2.32	0.70
3:C:199:MET:HA	3:C:199:MET:HE3	1.73	0.69
1:A:199:MET:HE3	1:A:199:MET:HA	1.73	0.69
1:A:327:MET:SD	1:A:335:VAL:CG1	2.81	0.69
2:B:368:ILE:HG22	2:B:476:THR:HG22	1.73	0.69
3:C:199:MET:CE	3:C:199:MET:HA	2.23	0.69
1:A:368:ILE:O	1:A:476:THR:HG21	1.92	0.68
3:C:298:PHE:HB3	3:C:318:LEU:HD23	1.75	0.68
1:A:298:PHE:HB3	1:A:318:LEU:HD23	1.75	0.68
1:A:295:VAL:O	1:A:320:LEU:HD12	1.94	0.68
2:B:199:MET:HA	2:B:199:MET:CE	2.24	0.68
1:A:348:LEU:HD11	1:A:510:ILE:CG2	2.23	0.67
4:D:249:ILE:HD12	4:D:316:MET:HE1	1.76	0.67
1:A:2256:UNK:CB	1:A:2262:UNK:HA	2.24	0.67
4:D:428:ILE:HD13	4:D:505:LEU:CD1	2.25	0.66
1:A:368:ILE:HG22	1:A:476:THR:HG22	1.76	0.66
2:B:298:PHE:HB3	2:B:318:LEU:HD23	1.75	0.66
2:B:295:VAL:O	2:B:320:LEU:HD12	1.95	0.66
2:B:204:LEU:HD22	2:B:313:VAL:HG11	1.78	0.66
2:B:291:GLU:OE1	2:B:293:LEU:HD21	1.97	0.65
3:C:295:VAL:O	3:C:320:LEU:HD12	1.95	0.65
1:A:199:MET:CE	1:A:199:MET:HA	2.26	0.65
1:A:363:PRO:HG3	1:A:476:THR:HG22	1.79	0.64
4:D:298:PHE:HB3	4:D:318:LEU:HD23	1.77	0.64
3:C:249:ILE:HD12	3:C:316:MET:HE2	1.79	0.64
1:A:507:ILE:HG22	1:A:508:ASP:O	1.98	0.64
2:B:348:LEU:HD11	2:B:510:ILE:CG2	2.27	0.64
4:D:204:LEU:HD22	4:D:313:VAL:HG11	1.78	0.64
1:A:31:ILE:HG21	1:A:359:LEU:CD1	2.27	0.64
4:D:521:VAL:HG12	4:D:1522:UNK:H	1.64	0.63
2:B:243:ILE:HD11	2:B:278:THR:HA	1.80	0.63
3:C:204:LEU:HD22	3:C:313:VAL:HG11	1.80	0.63
1:A:291:GLU:OE1	1:A:293:LEU:HD21	1.98	0.63
3:C:291:GLU:OE1	3:C:293:LEU:HD21	1.99	0.63
2:B:507:ILE:HG22	2:B:508:ASP:O	1.98	0.63
2:B:237:ALA:HB2	2:B:315:VAL:HG22	1.82	0.62
4:D:291:GLU:OE1	4:D:293:LEU:HD21	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:327:MET:SD	4:D:335:VAL:HG13	2.40	0.62
1:A:204:LEU:HD22	1:A:313:VAL:HG11	1.80	0.62
2:B:300:VAL:HG11	3:C:26:ILE:HD13	1.82	0.62
2:B:467:TYR:CG	2:B:503:ILE:HD11	2.34	0.62
3:C:243:ILE:HD11	3:C:278:THR:HA	1.81	0.61
1:A:382:ASN:C	1:A:1383:UNK:H	2.03	0.61
1:A:482:ALA:C	1:A:1483:UNK:H	2.04	0.61
2:B:199:MET:HE1	2:B:204:LEU:HD21	1.82	0.61
1:A:243:ILE:HD11	1:A:278:THR:HA	1.82	0.60
1:A:300:VAL:CG1	4:D:26:ILE:HD13	2.30	0.60
1:A:467:TYR:CG	1:A:503:ILE:HD11	2.37	0.60
4:D:199:MET:CE	4:D:204:LEU:HD11	2.32	0.59
1:A:349:ASN:OD1	1:A:350:ASP:N	2.35	0.59
1:A:232:ALA:HB3	1:A:320:LEU:HB3	1.83	0.59
1:A:238:GLY:O	1:A:241:VAL:HG23	2.02	0.59
4:D:236:ILE:HD11	4:D:249:ILE:CD1	2.18	0.59
4:D:264:PHE:HB3	4:D:280:THR:HG21	1.85	0.59
4:D:243:ILE:HD11	4:D:278:THR:HA	1.85	0.59
4:D:428:ILE:CD1	4:D:505:LEU:HD12	2.32	0.59
1:A:199:MET:HE1	1:A:204:LEU:HD21	1.83	0.59
4:D:295:VAL:O	4:D:320:LEU:HD12	2.01	0.59
4:D:359:LEU:HD23	4:D:505:LEU:HD22	1.85	0.59
2:B:349:ASN:OD1	2:B:350:ASP:N	2.35	0.59
2:B:424:ILE:HB	2:B:468:ILE:HG23	1.85	0.59
1:A:265:ILE:HD12	1:A:283:TYR:CD1	2.38	0.59
3:C:35:TYR:O	3:C:37:ARG:N	2.36	0.58
4:D:67:TYR:CE1	4:D:208:LEU:HD22	2.38	0.58
1:A:264:PHE:HB3	1:A:280:THR:HG21	1.85	0.58
2:B:306:LEU:HD22	2:B:311:ILE:HG21	1.85	0.58
2:B:482:ALA:C	2:B:1483:UNK:H	2.06	0.58
2:B:264:PHE:HB3	2:B:280:THR:HG21	1.85	0.58
3:C:264:PHE:HB3	3:C:280:THR:HG21	1.84	0.58
2:B:363:PRO:HG3	2:B:476:THR:HG22	1.86	0.58
4:D:306:LEU:HD22	4:D:311:ILE:HG21	1.86	0.58
3:C:199:MET:HE1	3:C:204:LEU:HD11	1.85	0.58
4:D:237:ALA:HB2	4:D:315:VAL:HG22	1.86	0.58
1:A:249:ILE:HD12	1:A:316:MET:CE	2.33	0.57
2:B:382:ASN:C	2:B:1383:UNK:H	2.05	0.57
3:C:506:LYS:N	3:C:1505:UNK:O	2.37	0.57
3:C:363:PRO:C	3:C:1364:UNK:N	2.57	0.57
3:C:67:TYR:CE1	3:C:208:LEU:HD22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ILE:HD12	2:B:316:MET:CE	2.35	0.57
1:A:424:ILE:HB	1:A:468:ILE:HG23	1.87	0.57
1:A:67:TYR:CE1	1:A:208:LEU:HD22	2.40	0.57
1:A:318:LEU:HD22	1:A:319:GLY:H	1.70	0.57
4:D:199:MET:HE1	4:D:204:LEU:HD11	1.85	0.56
1:A:1387:UNK:C	1:A:1389:UNK:H2	2.18	0.56
1:A:306:LEU:HD22	1:A:311:ILE:HG21	1.87	0.56
2:B:67:TYR:CE1	2:B:208:LEU:HD22	2.40	0.56
3:C:428:ILE:HA	3:C:437:GLY:HA2	1.87	0.56
4:D:1364:UNK:O	4:D:1365:UNK:C	2.53	0.56
2:B:351:ARG:HA	2:B:461:VAL:HG21	1.87	0.56
3:C:232:ALA:HB3	3:C:320:LEU:HB3	1.86	0.56
1:A:351:ARG:HA	1:A:461:VAL:HG21	1.88	0.56
2:B:428:ILE:HA	2:B:437:GLY:HA2	1.88	0.56
1:A:429:TYR:CD1	1:A:438:ILE:HD12	2.40	0.56
1:A:249:ILE:HD12	1:A:316:MET:HE1	1.88	0.56
1:A:176:ALA:HB3	2:B:178:SER:CB	2.34	0.56
3:C:199:MET:CE	3:C:204:LEU:HD11	2.36	0.56
2:B:278:THR:HG23	2:B:279:GLN:N	2.21	0.56
4:D:327:MET:SD	4:D:335:VAL:CG1	2.94	0.56
4:D:265:ILE:HD12	4:D:283:TYR:CD1	2.41	0.56
1:A:26:ILE:HD11	4:D:275:THR:OG1	2.05	0.55
2:B:265:ILE:HD12	2:B:283:TYR:CD1	2.41	0.55
1:A:213:ARG:HE	1:A:228:THR:CG2	2.18	0.55
2:B:429:TYR:CD1	2:B:438:ILE:HD12	2.41	0.55
2:B:327:MET:SD	2:B:335:VAL:HG13	2.46	0.55
4:D:337:GLU:HG2	4:D:344:TYR:CD2	2.42	0.55
2:B:1387:UNK:C	2:B:1389:UNK:H2	2.18	0.55
4:D:335:VAL:O	4:D:339:VAL:HG23	2.07	0.55
1:A:327:MET:SD	1:A:335:VAL:HG12	2.45	0.55
4:D:428:ILE:HA	4:D:437:GLY:HA2	1.89	0.55
1:A:428:ILE:HG23	1:A:463:THR:OG1	2.07	0.55
3:C:265:ILE:HD12	3:C:283:TYR:CD1	2.41	0.55
3:C:327:MET:SD	3:C:335:VAL:HG13	2.46	0.55
2:B:232:ALA:HB3	2:B:320:LEU:HB3	1.87	0.55
2:B:465:ILE:HG21	2:B:505:LEU:HD21	1.88	0.55
1:A:183:LEU:HD11	2:B:183:LEU:HD11	1.89	0.55
1:A:199:MET:CE	1:A:204:LEU:HD11	2.37	0.55
2:B:213:ARG:HE	2:B:228:THR:CG2	2.20	0.55
1:A:237:ALA:HB2	1:A:315:VAL:HG22	1.88	0.55
3:C:237:ALA:HB2	3:C:315:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ILE:HD12	2:B:316:MET:HE2	1.88	0.54
3:C:296:ALA:HB2	3:C:320:LEU:HD13	1.88	0.54
4:D:362:VAL:HG13	4:D:363:PRO:HD2	1.90	0.54
4:D:232:ALA:HB3	4:D:320:LEU:HB3	1.88	0.54
2:B:1386:UNK:O	2:B:1387:UNK:C	2.56	0.54
2:B:199:MET:CE	2:B:204:LEU:HD11	2.37	0.54
2:B:248:ALA:HB2	3:C:38:ILE:HG21	1.90	0.54
3:C:278:THR:HG23	3:C:279:GLN:N	2.22	0.54
4:D:357:VAL:HG11	4:D:428:ILE:HD11	1.90	0.54
3:C:318:LEU:HD22	3:C:319:GLY:H	1.72	0.54
1:A:295:VAL:O	1:A:320:LEU:CD1	2.56	0.54
2:B:35:TYR:O	2:B:38:ILE:N	2.34	0.54
1:A:178:SER:CB	2:B:176:ALA:HB3	2.39	0.53
3:C:35:TYR:O	3:C:36:PRO:C	2.46	0.53
4:D:226:LEU:HD21	4:D:336:ARG:HG2	1.90	0.53
2:B:318:LEU:HD22	2:B:319:GLY:H	1.74	0.53
1:A:428:ILE:HA	1:A:437:GLY:HA2	1.90	0.53
2:B:337:GLU:HG2	2:B:344:TYR:CD2	2.44	0.53
3:C:249:ILE:HD12	3:C:316:MET:CE	2.38	0.53
4:D:359:LEU:HD23	4:D:505:LEU:CD2	2.38	0.53
1:A:465:ILE:HG21	1:A:505:LEU:HD21	1.90	0.53
2:B:295:VAL:O	2:B:320:LEU:CD1	2.56	0.53
1:A:199:MET:HE1	1:A:204:LEU:HD11	1.91	0.53
1:A:265:ILE:HD12	1:A:283:TYR:CE1	2.43	0.53
2:B:265:ILE:HD12	2:B:283:TYR:CE1	2.44	0.53
2:B:226:LEU:HD21	2:B:336:ARG:HG2	1.90	0.53
4:D:249:ILE:HD12	4:D:316:MET:CE	2.38	0.53
2:B:199:MET:HE1	2:B:204:LEU:HD11	1.91	0.53
2:B:470:ALA:HB1	2:B:503:ILE:O	2.09	0.53
4:D:306:LEU:HD22	4:D:311:ILE:CG2	2.39	0.53
3:C:213:ARG:HE	3:C:228:THR:CG2	2.22	0.53
4:D:278:THR:HG23	4:D:279:GLN:N	2.23	0.52
3:C:337:GLU:HG2	3:C:344:TYR:CG	2.43	0.52
3:C:230:HIS:N	3:C:323:GLU:OE2	2.40	0.52
3:C:236:ILE:HD11	3:C:249:ILE:CD1	2.18	0.52
3:C:327:MET:SD	3:C:335:VAL:CG1	2.98	0.52
3:C:1364:UNK:O	3:C:1365:UNK:C	2.57	0.52
3:C:362:VAL:HG13	3:C:363:PRO:HD2	1.91	0.52
4:D:428:ILE:CD1	4:D:505:LEU:CD1	2.88	0.52
2:B:327:MET:SD	2:B:335:VAL:CG1	2.98	0.52
4:D:213:ARG:HE	4:D:228:THR:CG2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:MET:HE1	3:C:204:LEU:HD21	1.92	0.52
4:D:363:PRO:C	4:D:1364:UNK:N	2.63	0.52
1:A:521:VAL:HG12	1:A:522:ILE:N	2.25	0.52
1:A:26:ILE:CD1	4:D:275:THR:OG1	2.58	0.51
1:A:55:LEU:HD13	1:A:232:ALA:HB2	1.92	0.51
3:C:265:ILE:HD12	3:C:283:TYR:CE1	2.45	0.51
3:C:212:ASP:OD1	3:C:213:ARG:N	2.38	0.51
3:C:306:LEU:HD22	3:C:311:ILE:HG21	1.91	0.51
1:A:318:LEU:HD22	1:A:319:GLY:N	2.26	0.51
2:B:237:ALA:CB	2:B:315:VAL:HG22	2.40	0.51
2:B:428:ILE:HG23	2:B:463:THR:OG1	2.11	0.51
2:B:372:THR:HG21	2:B:473:PHE:CD1	2.46	0.51
1:A:372:THR:HG21	1:A:473:PHE:CD1	2.45	0.51
2:B:344:TYR:O	2:B:345:GLU:C	2.49	0.51
2:B:306:LEU:HD22	2:B:311:ILE:CG2	2.40	0.51
3:C:226:LEU:HD21	3:C:336:ARG:HG2	1.91	0.51
2:B:521:VAL:HG12	2:B:522:ILE:N	2.26	0.51
3:C:357:VAL:HG11	3:C:428:ILE:HD11	1.93	0.51
4:D:357:VAL:HG22	4:D:507:ILE:HG13	1.92	0.50
4:D:31:ILE:HG21	4:D:359:LEU:HD11	1.91	0.50
2:B:212:ASP:OD1	2:B:213:ARG:N	2.36	0.50
1:A:236:ILE:HD11	1:A:249:ILE:CD1	2.20	0.50
2:B:335:VAL:O	2:B:339:VAL:HG23	2.12	0.50
1:A:230:HIS:N	1:A:323:GLU:OE2	2.40	0.50
4:D:265:ILE:HD12	4:D:283:TYR:CE1	2.46	0.50
1:A:361:LYS:HG2	1:A:504:ASN:OD1	2.12	0.50
3:C:326:ALA:CB	3:C:338:MET:HE1	2.38	0.49
4:D:37:ARG:HA	4:D:355:SER:HA	1.95	0.49
1:A:1386:UNK:O	1:A:1387:UNK:C	2.59	0.49
1:A:22:THR:HG23	4:D:303:PRO:HG2	1.94	0.49
1:A:278:THR:HG23	1:A:279:GLN:N	2.26	0.49
2:B:348:LEU:HB2	2:B:514:GLN:OE1	2.12	0.49
2:B:326:ALA:CB	2:B:338:MET:HE1	2.42	0.49
3:C:318:LEU:HD22	3:C:319:GLY:N	2.28	0.49
1:A:380:VAL:HG22	1:A:468:ILE:HD13	1.94	0.49
1:A:61:ARG:CZ	3:C:60:LEU:HD13	2.41	0.49
2:B:296:ALA:HB2	2:B:320:LEU:HD13	1.94	0.49
4:D:31:ILE:HG21	4:D:359:LEU:CD1	2.42	0.49
4:D:362:VAL:CG1	4:D:363:PRO:HD2	2.43	0.49
4:D:197:ASP:O	4:D:201:LYS:HD2	2.13	0.49
2:B:55:LEU:HD13	2:B:232:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:VAL:O	3:C:320:LEU:CD1	2.61	0.49
1:A:212:ASP:OD1	1:A:213:ARG:N	2.39	0.49
1:A:296:ALA:HB2	1:A:320:LEU:HD13	1.94	0.48
2:B:35:TYR:O	2:B:37:ARG:N	2.46	0.48
1:A:197:ASP:O	1:A:201:LYS:HD2	2.13	0.48
2:B:361:LYS:HD2	2:B:474:LYS:HZ1	1.79	0.48
4:D:238:GLY:O	4:D:241:VAL:HG23	2.13	0.48
1:A:2272:UNK:O	1:A:2276:UNK:C	2.61	0.48
3:C:55:LEU:HD13	3:C:232:ALA:HB2	1.94	0.48
1:A:306:LEU:HD22	1:A:311:ILE:CG2	2.43	0.48
4:D:326:ALA:CB	4:D:338:MET:HE1	2.43	0.48
3:C:436:ILE:HD11	3:C:1456:UNK:CB	2.43	0.48
3:C:348:LEU:H	3:C:514:GLN:HE22	1.62	0.48
2:B:230:HIS:N	2:B:323:GLU:OE2	2.45	0.48
4:D:521:VAL:C	4:D:1522:UNK:H2	2.16	0.48
3:C:424:ILE:HG23	3:C:1528:UNK:CB	2.44	0.48
3:C:18:ALA:O	3:C:22:THR:HB	2.14	0.48
4:D:199:MET:HE1	4:D:204:LEU:HD21	1.95	0.48
4:D:31:ILE:O	4:D:37:ARG:NH1	2.47	0.48
4:D:318:LEU:HD22	4:D:319:GLY:H	1.77	0.48
2:B:318:LEU:HD22	2:B:319:GLY:N	2.27	0.47
3:C:357:VAL:HG22	3:C:507:ILE:HG13	1.96	0.47
1:A:426:ASN:HD22	1:A:426:ASN:N	2.13	0.47
1:A:248:ALA:HB2	4:D:38:ILE:HG21	1.96	0.47
1:A:226:LEU:HD21	1:A:336:ARG:HG2	1.95	0.47
3:C:197:ASP:O	3:C:201:LYS:HD2	2.14	0.47
2:B:238:GLY:O	2:B:241:VAL:HG23	2.15	0.47
4:D:296:ALA:HB2	4:D:320:LEU:HD13	1.96	0.47
4:D:436:ILE:HD11	4:D:1456:UNK:CB	2.45	0.47
1:A:326:ALA:CB	1:A:338:MET:CE	2.93	0.47
2:B:361:LYS:HG2	2:B:504:ASN:OD1	2.14	0.47
1:A:359:LEU:HD21	1:A:470:ALA:HA	1.97	0.47
1:A:368:ILE:HG22	1:A:476:THR:CG2	2.43	0.47
2:B:467:TYR:CD2	2:B:503:ILE:HD11	2.50	0.47
4:D:230:HIS:N	4:D:323:GLU:OE2	2.44	0.47
3:C:238:GLY:O	3:C:241:VAL:HG23	2.14	0.47
3:C:425:LEU:HD13	3:C:440:GLU:OE2	2.15	0.47
4:D:237:ALA:CB	4:D:315:VAL:HG22	2.45	0.47
1:A:503:ILE:HG23	1:A:505:LEU:HG	1.97	0.47
3:C:362:VAL:CG1	3:C:363:PRO:HD2	2.44	0.47
2:B:35:TYR:O	2:B:36:PRO:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:306:LEU:HD22	3:C:311:ILE:CG2	2.45	0.47
4:D:348:LEU:H	4:D:514:GLN:HE22	1.63	0.46
3:C:425:LEU:O	3:C:426:ASN:C	2.53	0.46
4:D:55:LEU:HD13	4:D:232:ALA:HB2	1.97	0.46
2:B:503:ILE:HG23	2:B:505:LEU:HG	1.97	0.46
1:A:18:ALA:O	1:A:22:THR:HB	2.14	0.46
1:A:354:ALA:HA	1:A:430:VAL:HG21	1.98	0.46
2:B:380:VAL:HG22	2:B:468:ILE:HD13	1.97	0.46
2:B:213:ARG:HE	2:B:228:THR:HG21	1.80	0.46
2:B:303:PRO:HG2	3:C:22:THR:HG23	1.97	0.46
2:B:197:ASP:O	2:B:201:LYS:HD2	2.15	0.45
2:B:244:ASN:HB3	3:C:38:ILE:HD12	1.98	0.45
1:A:326:ALA:HB1	1:A:338:MET:HE3	1.97	0.45
2:B:334:ASP:C	2:B:334:ASP:OD1	2.54	0.45
1:A:275:THR:OG1	4:D:26:ILE:HD12	2.16	0.45
4:D:505:LEU:HD21	4:D:1470:UNK:CB	2.47	0.45
2:B:326:ALA:HB3	2:B:338:MET:CE	2.44	0.45
1:A:213:ARG:HE	1:A:228:THR:HG21	1.80	0.45
2:B:186:HIS:HB3	2:B:188:THR:HG23	1.98	0.45
2:B:507:ILE:CG2	2:B:511:ALA:HB3	2.47	0.45
1:A:507:ILE:CG2	1:A:511:ALA:HB3	2.47	0.45
3:C:335:VAL:O	3:C:339:VAL:HG23	2.17	0.45
1:A:52:ILE:HG13	1:A:322:VAL:HG11	1.98	0.45
4:D:18:ALA:O	4:D:22:THR:HB	2.17	0.45
4:D:318:LEU:HD22	4:D:319:GLY:N	2.32	0.45
2:B:354:ALA:HA	2:B:430:VAL:HG21	1.98	0.45
2:B:222:ASP:OD1	2:B:225:HIS:N	2.50	0.45
2:B:60:LEU:HD13	4:D:61:ARG:CZ	2.47	0.45
3:C:52:ILE:HG13	3:C:322:VAL:HG11	1.97	0.45
4:D:295:VAL:O	4:D:320:LEU:CD1	2.65	0.44
3:C:237:ALA:CB	3:C:315:VAL:HG22	2.46	0.44
1:A:334:ASP:C	1:A:334:ASP:OD1	2.56	0.44
1:A:348:LEU:HB2	1:A:514:GLN:OE1	2.17	0.44
1:A:326:ALA:HB3	1:A:338:MET:CE	2.42	0.44
2:B:300:VAL:CG1	3:C:26:ILE:HD13	2.47	0.44
1:A:237:ALA:CB	1:A:315:VAL:HG22	2.47	0.44
3:C:2241:UNK:O	3:C:2242:UNK:C	2.65	0.44
4:D:56:ARG:HB3	4:D:211:ILE:HD13	2.00	0.44
4:D:428:ILE:HD12	4:D:505:LEU:HD12	1.99	0.44
2:B:336:ARG:HB3	2:B:344:TYR:OH	2.18	0.44
3:C:349:ASN:HB3	3:C:352:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:212:ASP:OD1	4:D:213:ARG:N	2.40	0.44
3:C:436:ILE:CD1	3:C:1456:UNK:CB	2.96	0.44
3:C:1463:UNK:O	3:C:1464:UNK:CB	2.66	0.44
2:B:426:ASN:N	2:B:426:ASN:HD22	2.16	0.44
2:B:326:ALA:CB	2:B:338:MET:CE	2.96	0.44
1:A:213:ARG:HE	1:A:228:THR:HG22	1.82	0.44
2:B:61:ARG:CZ	4:D:60:LEU:HD13	2.48	0.44
3:C:101:ARG:O	3:C:2210:UNK:C	2.66	0.43
2:B:292:TRP:O	2:B:293:LEU:HD23	2.17	0.43
3:C:1365:UNK:O	3:C:1366:UNK:C	2.66	0.43
3:C:31:ILE:HG21	3:C:359:LEU:HD11	2.00	0.43
4:D:48:VAL:CG2	4:D:338:MET:HE2	2.48	0.43
4:D:436:ILE:CD1	4:D:1456:UNK:CB	2.96	0.43
1:A:335:VAL:O	1:A:339:VAL:HG23	2.19	0.43
3:C:213:ARG:HE	3:C:228:THR:HG22	1.83	0.43
1:A:467:TYR:CD2	1:A:503:ILE:HD11	2.53	0.43
2:B:368:ILE:HG22	2:B:476:THR:CG2	2.44	0.43
1:A:186:HIS:HB3	1:A:188:THR:HG23	2.00	0.43
4:D:206:PHE:CE1	4:D:237:ALA:HB3	2.54	0.43
1:A:206:PHE:CE1	1:A:237:ALA:HB3	2.54	0.43
2:B:359:LEU:HD21	2:B:470:ALA:HA	2.01	0.43
3:C:512:LEU:O	3:C:513:LYS:C	2.57	0.43
4:D:348:LEU:CD1	4:D:510:ILE:HG22	2.49	0.42
4:D:434:ASN:HD22	4:D:521:VAL:H	1.67	0.42
2:B:207:LYS:O	2:B:208:LEU:HD23	2.18	0.42
1:A:22:THR:CG2	4:D:303:PRO:HD2	2.50	0.42
3:C:101:ARG:HH12	3:C:2248:UNK:CB	2.33	0.42
1:A:470:ALA:HB1	1:A:503:ILE:O	2.19	0.42
2:B:357:VAL:HG22	2:B:507:ILE:HG12	2.02	0.42
1:A:361:LYS:HD2	1:A:474:LYS:HZ1	1.85	0.42
2:B:361:LYS:HE3	2:B:474:LYS:HZ2	1.85	0.42
4:D:349:ASN:HB3	4:D:352:ASN:ND2	2.34	0.42
1:A:62:MET:CE	1:A:252:GLY:HA3	2.50	0.42
4:D:48:VAL:HG23	4:D:338:MET:HE2	2.01	0.42
2:B:52:ILE:HG13	2:B:322:VAL:HG11	2.00	0.42
1:A:249:ILE:HD12	1:A:316:MET:HE3	2.02	0.42
3:C:326:ALA:CB	3:C:338:MET:CE	2.98	0.42
3:C:206:PHE:CE1	3:C:237:ALA:HB3	2.55	0.42
1:A:2254:UNK:O	1:A:2258:UNK:CB	2.67	0.42
3:C:186:HIS:HB3	3:C:188:THR:HG23	2.02	0.42
3:C:292:TRP:O	3:C:293:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:OD1	1:A:225:HIS:N	2.53	0.41
1:A:503:ILE:HG21	1:A:505:LEU:HD12	2.02	0.41
4:D:1365:UNK:O	4:D:1366:UNK:C	2.68	0.41
1:A:242:ASP:OD2	1:A:244:ASN:ND2	2.53	0.41
1:A:479:LEU:O	1:A:1483:UNK:N	2.54	0.41
2:B:479:LEU:O	2:B:1483:UNK:N	2.53	0.41
2:B:48:VAL:CG2	2:B:338:MET:HE2	2.50	0.41
2:B:253:LEU:HD23	2:B:320:LEU:HD22	2.03	0.41
1:A:26:ILE:HD13	4:D:300:VAL:HG11	2.02	0.41
2:B:423:SER:HB2	2:B:426:ASN:HD21	1.86	0.41
2:B:62:MET:HG2	3:C:42:PHE:HB3	2.03	0.41
4:D:326:ALA:CB	4:D:338:MET:CE	2.98	0.41
4:D:213:ARG:HE	4:D:228:THR:HG22	1.83	0.41
3:C:10:MET:HG2	3:C:18:ALA:HB2	2.03	0.41
2:B:303:PRO:HD2	3:C:22:THR:CG2	2.51	0.41
1:A:303:PRO:HD2	4:D:22:THR:CG2	2.51	0.41
4:D:1463:UNK:O	4:D:1464:UNK:CB	2.68	0.41
4:D:222:ASP:OD1	4:D:225:HIS:N	2.54	0.41
3:C:348:LEU:CD1	3:C:510:ILE:HG22	2.51	0.41
3:C:46:HIS:CG	3:C:47:PRO:HD2	2.56	0.41
1:A:97:ALA:HB2	2:B:97:ALA:HB2	2.03	0.41
2:B:503:ILE:HG21	2:B:505:LEU:HD12	2.02	0.40
1:A:372:THR:HG21	1:A:473:PHE:CG	2.56	0.40
3:C:62:MET:CE	3:C:252:GLY:HA3	2.51	0.40
2:B:213:ARG:NE	2:B:228:THR:HG21	2.35	0.40
3:C:431:TYR:O	3:C:432:ASP:C	2.59	0.40
2:B:436:ILE:HA	2:B:1523:UNK:H	1.86	0.40
1:A:213:ARG:NE	1:A:228:THR:HG21	2.36	0.40
4:D:186:HIS:HB3	4:D:188:THR:HG23	2.02	0.40
2:B:56:ARG:HB3	2:B:211:ILE:HD13	2.03	0.40
4:D:45:THR:HG23	4:D:50:ASP:OD2	2.22	0.40
3:C:182:THR:CG2	3:C:183:LEU:N	2.85	0.40
4:D:215:PHE:CE2	4:D:228:THR:HG23	2.57	0.40

All (1) 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)
2:B:220:LYS:NZ	4:D:518:LYS:CD[3_655]	1.94	0.26

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	372/665 (56%)	345 (93%)	24 (6%)	3 (1%)	24	69
2	B	346/648 (53%)	320 (92%)	22 (6%)	4 (1%)	16	60
3	C	315/701 (45%)	283 (90%)	27 (9%)	5 (2%)	12	54
4	D	315/685 (46%)	287 (91%)	26 (8%)	2 (1%)	30	75
All	All	1348/2699 (50%)	1235 (92%)	99 (7%)	14 (1%)	19	64

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
2	B	35	TYR
2	B	349	ASN
3	C	35	TYR
3	C	426	ASN
3	C	432	ASP
1	A	276	PRO
2	B	276	PRO
3	C	276	PRO
4	D	276	PRO
1	A	295	VAL
2	B	295	VAL
3	C	295	VAL
4	D	295	VAL

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	339/497 (68%)	313 (92%)	26 (8%)	16 54
2	B	316/497 (64%)	291 (92%)	25 (8%)	15 52
3	C	286/497 (58%)	260 (91%)	26 (9%)	12 42
4	D	286/498 (57%)	261 (91%)	25 (9%)	13 45
All	All	1227/1989 (62%)	1125 (92%)	102 (8%)	14 49

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	37	ARG
1	A	80	LYS
1	A	171	PHE
1	A	180	LYS
1	A	188	THR
1	A	197	ASP
1	A	199	MET
1	A	206	PHE
1	A	217	ARG
1	A	239	GLU
1	A	278	THR
1	A	318	LEU
1	A	325	LEU
1	A	336	ARG
1	A	342	GLN
1	A	350	ASP
1	A	351	ARG
1	A	371	LEU
1	A	426	ASN
1	A	429	TYR
1	A	434	ASN
1	A	463	THR
1	A	468	ILE
1	A	474	LYS
1	A	481	GLU
2	B	37	ARG
2	B	39	LYS
2	B	80	LYS
2	B	171	PHE
2	B	180	LYS
2	B	188	THR
2	B	197	ASP

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Mol	Chain	Res	Type
2	B	199	MET
2	B	206	PHE
2	B	217	ARG
2	B	239	GLU
2	B	318	LEU
2	B	325	LEU
2	B	342	GLN
2	B	350	ASP
2	B	351	ARG
2	B	371	LEU
2	B	426	ASN
2	B	429	TYR
2	B	434	ASN
2	B	463	THR
2	B	468	ILE
2	B	474	LYS
2	B	481	GLU
2	B	502	ASP
3	C	22	THR
3	C	37	ARG
3	C	38	ILE
3	C	80	LYS
3	C	171	PHE
3	C	180	LYS
3	C	188	THR
3	C	197	ASP
3	C	199	MET
3	C	206	PHE
3	C	217	ARG
3	C	239	GLU
3	C	278	THR
3	C	318	LEU
3	C	325	LEU
3	C	336	ARG
3	C	342	GLN
3	C	345	GLU
3	C	350	ASP
3	C	351	ARG
3	C	361	LYS
3	C	424	ILE
3	C	428	ILE
3	C	434	ASN

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Mol	Chain	Res	Type
3	C	507	ILE
3	C	512	LEU
4	D	22	THR
4	D	37	ARG
4	D	80	LYS
4	D	171	PHE
4	D	180	LYS
4	D	188	THR
4	D	197	ASP
4	D	199	MET
4	D	206	PHE
4	D	217	ARG
4	D	239	GLU
4	D	243	ILE
4	D	278	THR
4	D	318	LEU
4	D	325	LEU
4	D	342	GLN
4	D	345	GLU
4	D	350	ASP
4	D	351	ARG
4	D	361	LYS
4	D	428	ILE
4	D	434	ASN
4	D	507	ILE
4	D	512	LEU
4	D	521	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	286	HIS
1	A	342	GLN
1	A	426	ASN
2	B	57	GLN
2	B	256	GLN
2	B	342	GLN
2	B	426	ASN
3	C	286	HIS
3	C	342	GLN
4	D	286	HIS

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Mol	Chain	Res	Type
4	D	342	GLN
4	D	352	ASN
4	D	434	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

There are no ligands in this entry.

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	382/665 (57%)	0.80	36 (9%) 11 7	132, 140, 141, 144	0
2	B	356/648 (54%)	0.81	42 (11%) 6 4	130, 140, 141, 147	0
3	C	323/701 (46%)	0.98	48 (14%) 3 2	126, 140, 141, 157	0
4	D	323/685 (47%)	0.94	32 (9%) 9 6	126, 140, 141, 146	0
All	All	1384/2699 (51%)	0.88	158 (11%) 7 4	126, 140, 141, 157	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	273	TYR	7.6
3	C	436	ILE	7.1
1	A	436	ILE	6.7
3	C	431	TYR	6.6
4	D	362	VAL	5.9
3	C	91	ASP	5.9
2	B	312	ASP	5.7
2	B	452	PHE	5.5
1	A	19	TRP	5.0
1	A	7	ILE	4.4
1	A	16	GLU	4.4
4	D	363	PRO	4.4
4	D	1481	GLU	4.3
4	D	99	LEU	4.2
1	A	18	ALA	4.1
3	C	271	SER	4.1
2	B	431	TYR	4.0
1	A	15	PHE	4.0
4	D	189	SER	4.0
3	C	434	ASN	4.0
1	A	219	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	346	HIS	3.9
2	B	348	LEU	3.7
4	D	431	TYR	3.6
4	D	439	PRO	3.6
3	C	507	ILE	3.6
3	C	7	ILE	3.6
4	D	13	LYS	3.5
2	B	357	VAL	3.5
1	A	26	ILE	3.4
2	B	362	VAL	3.4
4	D	515	ILE	3.3
2	B	95	TYR	3.3
4	D	430	VAL	3.3
1	A	304	VAL	3.2
3	C	435	VAL	3.2
4	D	440	GLU	3.2
4	D	361	LYS	3.2
1	A	348	LEU	3.1
3	C	424	ILE	3.1
4	D	436	ILE	3.0
4	D	507	ILE	3.0
3	C	298	PHE	3.0
2	B	35	TYR	3.0
3	C	221	GLU	3.0
2	B	353	VAL	3.0
1	A	465	ILE	3.0
1	A	368	ILE	3.0
2	B	220	LYS	3.0
1	A	345	GLU	3.0
2	B	467	TYR	2.9
4	D	7	ILE	2.9
4	D	438	ILE	2.9
2	B	435	VAL	2.9
1	A	503	ILE	2.9
2	B	449	PHE	2.9
1	A	357	VAL	2.9
2	B	456	GLY	2.9
3	C	440	GLU	2.9
3	C	22	THR	2.8
3	C	35	TYR	2.8
3	C	204	LEU	2.8
4	D	348	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	304	VAL	2.8
4	D	31	ILE	2.8
2	B	454	GLU	2.8
3	C	313	VAL	2.8
4	D	299	GLY	2.8
1	A	440	GLU	2.8
1	A	293	LEU	2.8
4	D	94	PHE	2.8
1	A	510	ILE	2.7
3	C	433	GLY	2.7
1	A	435	VAL	2.7
2	B	423	SER	2.7
2	B	289	LEU	2.7
3	C	272	LYS	2.7
1	A	479	LEU	2.7
4	D	26	ILE	2.7
3	C	19	TRP	2.7
4	D	172	LYS	2.6
2	B	176	ALA	2.6
3	C	87	MET	2.6
3	C	270	LYS	2.6
3	C	285	TYR	2.6
2	B	428	ILE	2.6
2	B	303	PRO	2.6
4	D	223	LYS	2.6
3	C	174	LEU	2.5
1	A	220	LYS	2.5
1	A	101	ARG	2.5
4	D	293	LEU	2.5
3	C	515	ILE	2.5
4	D	260	THR	2.5
2	B	453	LEU	2.5
3	C	192	PHE	2.5
3	C	347	LYS	2.5
3	C	292	TRP	2.5
2	B	292	TRP	2.5
1	A	20	ILE	2.4
1	A	521	VAL	2.4
2	B	259	PHE	2.4
3	C	315	VAL	2.4
1	A	452	PHE	2.4
1	A	365	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	90	LEU	2.4
3	C	84	PRO	2.4
4	D	259	PHE	2.4
2	B	333	ALA	2.4
1	A	189	SER	2.4
4	D	298	PHE	2.4
2	B	359	LEU	2.4
2	B	272	LYS	2.4
2	B	506	LYS	2.4
3	C	321	GLY	2.4
4	D	516	MET	2.3
3	C	171	PHE	2.3
1	A	336	ARG	2.3
3	C	95	TYR	2.3
3	C	361	LYS	2.3
1	A	359	LEU	2.3
3	C	301	TYR	2.3
1	A	515	ILE	2.3
3	C	348	LEU	2.3
1	A	9	GLU	2.3
3	C	191	TRP	2.3
1	A	10	MET	2.3
1	A	321	GLY	2.3
2	B	436	ILE	2.3
2	B	84	PRO	2.2
2	B	244	ASN	2.2
2	B	100	PRO	2.2
3	C	316	MET	2.2
2	B	502	ASP	2.2
2	B	284	ALA	2.2
3	C	280	THR	2.2
3	C	73	VAL	2.2
3	C	17	LYS	2.1
2	B	192	PHE	2.1
1	A	362	VAL	2.1
3	C	26	ILE	2.1
2	B	450	LYS	2.1
4	D	353	VAL	2.1
3	C	425	LEU	2.1
2	B	293	LEU	2.1
4	D	244	ASN	2.1
2	B	308	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	359	LEU	2.1
3	C	295	VAL	2.1
2	B	31	ILE	2.1
4	D	219	GLN	2.1
2	B	295	VAL	2.1
4	D	8	ILE	2.0
2	B	96	LEU	2.0
1	A	456	GLY	2.0
3	C	82	PHE	2.0
3	C	206	PHE	2.0
2	B	49	ASN	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.