Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:23 AM GMT

PDB ID	:	2CV2
Title	:	Glutamyl-tRNA synthetase from Thermus thermophilus in complex with tRNA(Glu) and an enzyme inhibitor, Glu-AMS
Authors	:	Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-31
Resolution	:	2.69 Å(reported)

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 2.69 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		15
Ramachandran outliers		0.3%
Sidechain outliers		8.1%
RSRZ outliers		1.8%
RNA backbone		0.65

Worse   *Better*

▮ Percentile relative to all X-ray structures
❘ Percentile relative to X-ray structures of similar resolution
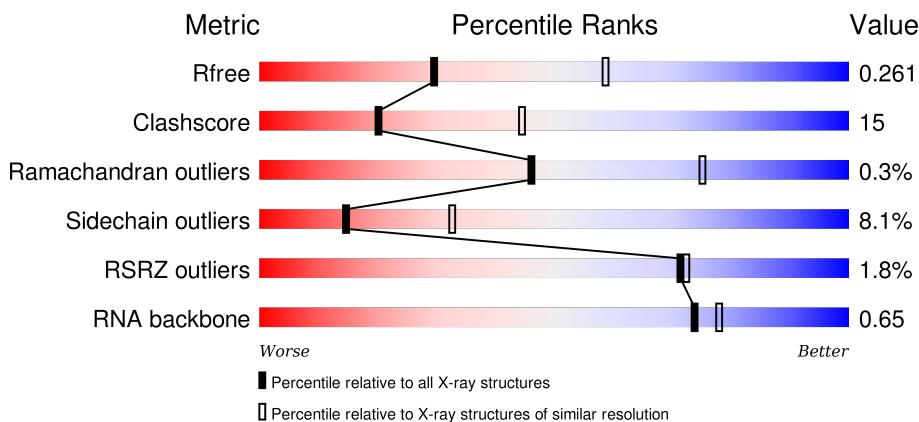
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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	C	75	3% — 52% / 32% / 12% / •
1	D	75	3% — 53% / 31% / 12% / •
2	A	468	% — 68% / 29% / •
2	B	468	2% — 61% / 34% / 5%
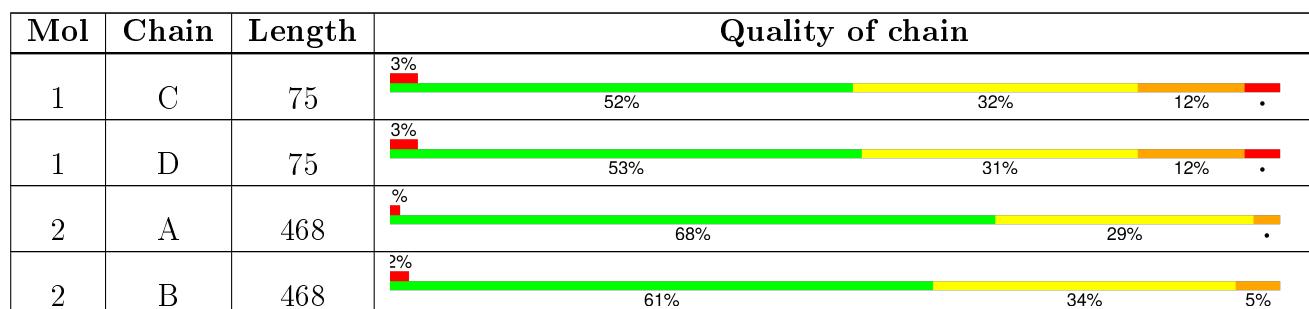
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	904	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11215 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			
1	D	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			
2	B	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 5 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: $C_{15}H_{21}N_7O_9S$).
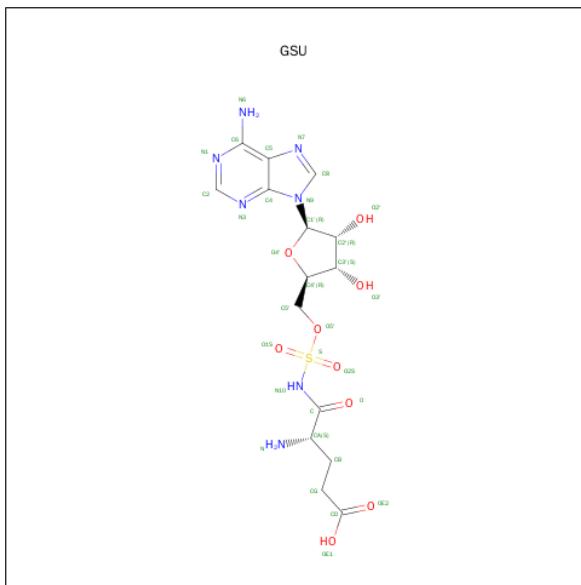
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			32	15	7	9	1		
5	B	1	Total	C	N	O	S	0	0
			32	15	7	9	1		

• Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	116	Total	O	0	0
			116	116		
6	C	48	Total	O	0	0
			48	48		
6	D	36	Total	O	0	0
			36	36		

3 Residue-property plots ⓘ

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: tRNA
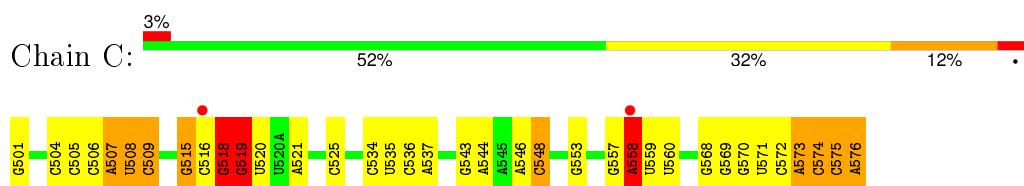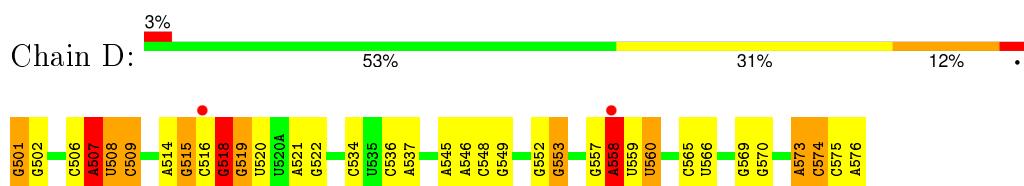
Chain C:

- Molecule 1: tRNA

Chain D:

- Molecule 2: glutamyl-tRNA synthetase

Chain A:

- Molecule 2: glutamyl-tRNA synthetase

Chain B:
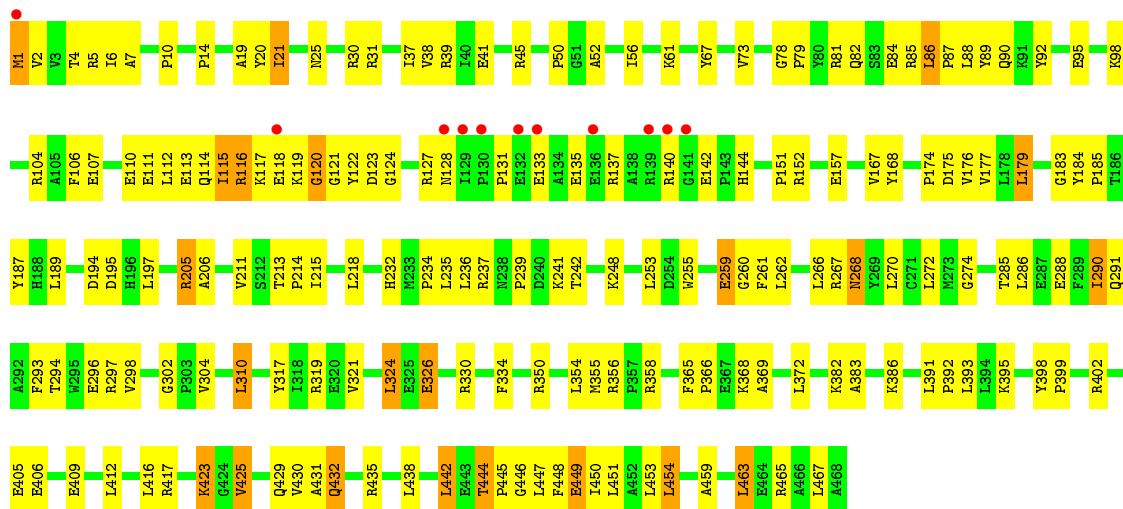
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.32Å 219.82Å 135.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 2.69 46.34 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.34-2.69) 96.4 (46.34-2.63)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.260 0.201 , 0.261	Depositor DCC
R_{free} test set	2300 reflections (5.01%)	DCC
Wilson B-factor (Å²)	40.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 47476 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GSU, 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	C	0.55	1/1782 (0.1%)	0.86	9/2774 (0.3%)
1	D	0.54	1/1782 (0.1%)	0.87	9/2774 (0.3%)
2	A	0.52	0/3910	0.70	0/5293
2	B	0.52	0/3910	0.68	0/5293
All	All	0.53	2/11384 (0.0%)	0.75	18/16134 (0.1%)

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	C	1	3
1	D	1	3
All	All	2	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.12	1.52	1.61
1	D	501	G	OP3-P	-5.85	1.54	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	A	C2'-C3'-O3'	8.16	127.46	109.50
1	C	558	A	C2'-C3'-O3'	7.83	126.72	109.50
1	D	507	A	C2'-C3'-O3'	7.76	126.56	109.50
1	C	573	A	C2'-C3'-O3'	7.31	125.58	109.50
1	D	573	A	C2'-C3'-O3'	7.30	125.57	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	518	G	C2'-C3'-O3'	7.17	125.26	109.50
1	C	519	G	C2'-C3'-O3'	7.06	125.03	109.50
1	C	518	G	C2'-C3'-O3'	7.02	124.94	109.50
1	D	509	C	N1-C1'-C2'	6.92	123.00	114.00
1	D	519	G	C2'-C3'-O3'	6.77	124.53	113.70
1	C	509	C	N1-C1'-C2'	6.55	122.52	114.00
1	C	548	C	N1-C1'-C2'	6.54	122.51	114.00
1	D	558	A	C4'-C3'-C2'	5.96	108.56	102.60
1	C	558	A	C4'-C3'-C2'	5.88	108.48	102.60
1	D	507	A	C4'-C3'-C2'	5.73	108.33	102.60
1	C	576	A	C2'-C3'-O3'	5.49	122.48	113.70
1	D	518	G	C4'-C3'-C2'	5.13	107.73	102.60
1	C	558	A	C4'-C3'-O3'	5.04	123.08	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	558	A	C3'
1	D	558	A	C3'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	C	535	U	Sidechain
1	C	568	G	Sidechain
1	D	515	G	Sidechain
1	D	522	G	Sidechain
1	D	545	A	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	C	1597	0	813	19	0
1	D	1597	0	813	19	0
2	A	3814	0	3818	115	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3814	0	3818	157	1
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	32	0	20	2	0
5	B	32	0	20	2	0
6	A	125	0	0	6	0
6	B	116	0	0	6	0
6	C	48	0	0	0	0
6	D	36	0	0	0	0
All	All	11215	0	9302	297	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 15.

All (297) 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)
2:A:247:ARG:HD3	2:A:247:ARG:H	1.29	0.96
2:A:177:VAL:HG23	2:A:186:THR:HG21	1.49	0.95
2:A:163:ARG:HH12	2:A:300:LEU:HD22	1.31	0.92
2:B:454:LEU:H	2:B:454:LEU:HD22	1.38	0.86
2:B:435:ARG:HH11	2:B:444:THR:CG2	1.89	0.85
1:D:574:C:H5"	2:B:177:VAL:HG21	1.61	0.82
1:C:518:G:O2'	1:C:557:G:N2	2.12	0.82
2:B:454:LEU:N	2:B:454:LEU:HD22	1.94	0.82
2:A:163:ARG:NH1	2:A:300:LEU:HD13	1.95	0.81
2:A:163:ARG:HH11	2:A:300:LEU:HD13	1.45	0.80
2:A:152:ARG:HH11	2:A:152:ARG:HG2	1.47	0.78
1:D:576:A:H5"	2:B:187:TYR:HB2	1.65	0.77
1:D:506:C:O2'	1:D:507:A:H5'	1.85	0.77
2:B:438:LEU:HD11	2:B:451:LEU:HD13	1.66	0.76
2:A:446:GLY:O	2:A:449:GLU:HG2	1.86	0.75
2:B:137:ARG:HB3	2:B:142:GLU:OE1	1.86	0.75
2:B:435:ARG:HH11	2:B:444:THR:HG22	1.50	0.74
2:A:267:ARG:HD2	2:A:286:LEU:HG	1.70	0.73
2:A:177:VAL:HG23	2:A:186:THR:CG2	2.19	0.73
2:B:365:PHE:HB3	2:B:366:PRO:HD3	1.71	0.73
1:D:570:G:H21	2:B:211:VAL:HG11	1.55	0.72
2:B:398:TYR:HB3	2:B:399:PRO:HD3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:ARG:HH11	2:B:465:ARG:HB3	1.55	0.71
2:B:4:THR:HB	2:B:25:ASN:HD22	1.55	0.71
2:B:261:PHE:CE2	2:B:310:LEU:HD13	2.27	0.69
2:A:361:THR:OG1	2:A:364:GLU:HG3	1.94	0.68
2:B:435:ARG:HD3	2:B:444:THR:HG22	1.77	0.66
2:A:152:ARG:NH1	2:A:152:ARG:HG2	2.08	0.66
2:B:104:ARG:HB3	2:B:144:HIS:HD2	1.59	0.66
2:A:333:PRO:HA	2:A:336:ARG:NH1	2.11	0.66
2:A:37:ILE:HD12	2:A:69:GLU:HB2	1.77	0.65
2:A:255:TRP:CZ2	2:A:259:GLU:HG3	2.31	0.65
2:B:444:THR:HG23	2:B:445:PRO:O	1.96	0.65
2:B:205:ARG:HD3	2:B:232:HIS:NE2	2.12	0.65
2:B:50:PRO:HB3	6:B:1209:HOH:O	1.96	0.65
2:B:454:LEU:HD13	2:B:454:LEU:H	1.62	0.64
1:D:518:G:O2'	1:D:557:G:N2	2.31	0.64
2:A:297:ARG:HH11	2:A:297:ARG:HG2	1.62	0.64
2:B:386:LYS:HE2	2:B:432:GLN:HG2	1.80	0.64
2:B:454:LEU:CD2	2:B:454:LEU:H	2.02	0.63
2:B:450:ILE:O	2:B:454:LEU:HD11	1.99	0.62
2:B:112:LEU:O	2:B:115:ILE:HD13	2.00	0.62
2:A:5:ARG:HB3	2:A:37:ILE:HB	1.82	0.62
1:C:570:G:H21	2:A:211:VAL:HG11	1.64	0.62
2:A:61:LYS:HG2	6:A:1183:HOH:O	1.99	0.62
2:B:6:ILE:CD1	2:B:21:ILE:HG22	2.29	0.61
2:A:393:LEU:H	2:A:393:LEU:HD23	1.62	0.61
2:B:454:LEU:N	2:B:454:LEU:HD13	2.14	0.61
2:A:163:ARG:HH12	2:A:300:LEU:CD2	2.10	0.61
2:B:157:GLU:HG2	2:B:167:VAL:HG22	1.83	0.61
2:B:294:THR:CG2	2:B:297:ARG:HG2	2.31	0.61
2:B:39:ARG:NH2	2:B:195:ASP:OD2	2.34	0.60
2:B:317:TYR:HA	2:B:321:VAL:HG23	1.84	0.60
2:A:406:GLU:O	2:A:406:GLU:HG3	2.02	0.60
2:A:207:GLU:HG2	6:A:1150:HOH:O	2.01	0.59
2:B:248:LYS:HD3	6:B:1301:HOH:O	2.01	0.59
2:B:116:ARG:O	2:B:120:GLY:HA2	2.02	0.59
2:B:39:ARG:NH1	2:B:41:GLU:OE1	2.32	0.59
2:B:31:ARG:NH1	2:B:293:PHE:O	2.34	0.59
2:A:177:VAL:CG2	2:A:186:THR:HG21	2.27	0.59
2:B:114:GLN:O	2:B:118:GLU:HG2	2.03	0.59
2:B:358:ARG:O	2:B:368:LYS:HE2	2.01	0.59
2:A:261:PHE:CE2	2:A:310:LEU:HD13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:458:ARG:HD3	2:A:461:ARG:HH21	1.68	0.58
2:A:400:ARG:HH22	2:A:422:GLU:CD	2.06	0.58
2:A:247:ARG:CD	2:A:247:ARG:H	2.04	0.58
2:A:247:ARG:HD3	2:A:247:ARG:N	2.11	0.58
2:B:179:LEU:HD23	2:B:184:TYR:O	2.03	0.58
2:B:391:LEU:N	2:B:392:PRO:HD2	2.18	0.58
2:B:285:THR:OG1	2:B:288:GLU:HG3	2.03	0.58
2:A:205:ARG:HD3	2:A:232:HIS:NE2	2.19	0.57
2:A:18:THR:HG21	2:A:56:ILE:HD11	1.85	0.57
2:A:82:GLN:NE2	2:A:190:ALA:HB1	2.20	0.57
2:A:350:ARG:NH2	2:A:409:GLU:OE1	2.38	0.57
2:B:10:PRO:HB3	2:B:52:ALA:HB3	1.86	0.57
2:A:297:ARG:NH1	2:A:297:ARG:HG2	2.20	0.56
2:B:7:ALA:HB1	2:B:41:GLU:HG3	1.87	0.56
2:B:290:ILE:HD12	2:B:290:ILE:C	2.25	0.56
2:A:285:THR:OG1	2:A:288:GLU:HG3	2.05	0.56
2:A:445:PRO:HG2	2:A:450:ILE:HD11	1.86	0.56
2:B:444:THR:OG1	2:B:445:PRO:HD2	2.05	0.56
2:B:319:ARG:HD2	6:B:1006:HOH:O	2.05	0.56
2:B:326:GLU:O	2:B:330:ARG:HG3	2.05	0.56
2:B:111:GLU:O	2:B:115:ILE:HG23	2.06	0.56
2:B:6:ILE:HG23	2:B:6:ILE:O	2.06	0.56
2:B:402:ARG:HH11	2:B:402:ARG:HG2	1.71	0.55
2:B:435:ARG:NH1	2:B:444:THR:HG22	2.20	0.55
2:B:25:ASN:ND2	6:B:1009:HOH:O	2.39	0.55
2:B:423:LYS:HZ3	2:B:423:LYS:HB2	1.72	0.55
2:A:420:ALA:HB1	2:A:425:VAL:O	2.05	0.55
2:B:465:ARG:NH1	2:B:465:ARG:HB3	2.20	0.55
1:D:558:A:O2'	1:D:560:U:OP2	2.22	0.55
2:B:431:ALA:HB1	2:B:447:LEU:HD22	1.89	0.55
2:A:37:ILE:HD13	2:A:37:ILE:N	2.21	0.55
2:B:237:ARG:NH1	2:B:302:GLY:HA3	2.22	0.54
2:B:110:GLU:O	2:B:114:GLN:HG2	2.08	0.54
2:A:283:ILE:HD13	2:A:313:MET:HE2	1.90	0.54
1:C:574:C:H5"	2:A:177:VAL:HG11	1.90	0.54
2:B:52:ALA:O	2:B:56:ILE:HG22	2.07	0.54
2:B:416:LEU:HD12	2:B:448:PHE:HE1	1.72	0.54
2:B:454:LEU:CD1	2:B:454:LEU:H	2.19	0.53
2:A:267:ARG:NH2	2:A:284:PHE:O	2.39	0.53
2:B:168:TYR:CD2	2:B:214:PRO:HG3	2.43	0.53
1:D:574:C:H5	2:B:112:LEU:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:44:ASP:OD1	2:A:47:ARG:HG3	2.09	0.53
2:B:45:ARG:HD3	2:B:184:TYR:CE2	2.44	0.53
2:A:21:ILE:HG13	5:A:601:GSU:H1'	1.89	0.53
2:A:163:ARG:NH2	2:A:232:HIS:O	2.42	0.53
2:B:235:LEU:O	2:B:237:ARG:HD3	2.08	0.53
2:B:435:ARG:HD3	2:B:444:THR:CG2	2.38	0.53
2:A:255:TRP:CH2	2:A:259:GLU:HG3	2.44	0.52
2:A:116:ARG:HG3	2:A:121:GLY:H	1.73	0.52
1:C:558:A:O2'	1:C:560:U:OP2	2.23	0.52
2:A:62:TRP:CE2	2:A:263:PRO:HB3	2.44	0.52
1:D:534:C:O2	2:B:435:ARG:NH2	2.37	0.52
2:A:245:SER:HB2	2:A:247:ARG:CZ	2.39	0.51
2:A:463:LEU:HD23	2:A:463:LEU:O	2.10	0.51
2:A:206:ALA:HB1	2:A:235:LEU:HD13	1.90	0.51
2:A:16:VAL:HG13	2:A:251:THR:O	2.10	0.51
2:B:326:GLU:HA	2:B:326:GLU:OE2	2.10	0.51
2:A:319:ARG:HG3	2:A:320:GLU:HG3	1.93	0.51
2:B:19:ALA:HB2	2:B:253:LEU:HD11	1.92	0.51
2:B:61:LYS:HE3	2:B:67:TYR:OH	2.11	0.51
2:A:365:PHE:HB3	2:A:366:PRO:HD3	1.92	0.51
2:A:136:GLU:HG2	2:A:139:ARG:NH1	2.26	0.51
2:A:294:THR:HG23	2:A:296:GLU:H	1.76	0.50
2:B:260:GLY:HA2	2:B:334:PHE:CZ	2.47	0.50
1:C:519:G:N2	1:C:557:G:H1'	2.27	0.50
2:B:290:ILE:HG13	2:B:291:GLN:N	2.27	0.50
2:A:445:PRO:CG	2:A:450:ILE:HD11	2.42	0.50
1:C:506:C:O2'	1:C:507:A:H5'	2.11	0.50
2:A:116:ARG:O	2:A:120:GLY:HA2	2.11	0.50
2:A:140:ARG:HG2	2:A:140:ARG:HH11	1.76	0.50
2:B:268:ASN:C	2:B:268:ASN:HD22	2.14	0.50
2:B:267:ARG:HD2	2:B:286:LEU:HB2	1.93	0.50
2:B:89:TYR:CD2	2:B:185:PRO:HG3	2.47	0.50
2:A:416:LEU:HD12	2:A:448:PHE:HE1	1.77	0.50
1:D:569:G:H5"	2:B:242:THR:HA	1.93	0.50
2:A:458:ARG:HH11	2:A:461:ARG:NH2	2.10	0.50
2:A:205:ARG:HG3	2:A:209:TRP:CD1	2.46	0.49
1:C:505:C:O3'	2:A:163:ARG:HD3	2.12	0.49
2:A:458:ARG:HD3	2:A:461:ARG:NH2	2.26	0.49
2:B:382:LYS:HB3	2:B:382:LYS:NZ	2.27	0.49
2:A:213:THR:N	2:A:214:PRO:HD2	2.28	0.49
2:B:425:VAL:HG22	2:B:429:GLN:CD	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:26:TYR:CE1	2:A:290:ILE:HD11	2.47	0.49
2:B:416:LEU:HD12	2:B:448:PHE:CE1	2.48	0.49
2:B:187:TYR:CE1	5:B:602:GSU:HG2	2.48	0.49
2:B:431:ALA:CB	2:B:447:LEU:HD22	2.43	0.49
2:B:137:ARG:O	2:B:142:GLU:HB3	2.12	0.49
2:B:294:THR:HG23	2:B:294:THR:O	2.12	0.49
2:A:7:ALA:HA	2:A:39:ARG:O	2.12	0.49
2:B:116:ARG:HA	2:B:121:GLY:H	1.78	0.48
1:C:576:A:O3'	5:A:601:GSU:N	2.46	0.48
2:B:37:ILE:HG22	2:B:38:VAL:N	2.26	0.48
1:D:521:A:H61	1:D:546:A:H2'	1.79	0.48
2:B:454:LEU:HD23	2:B:459:ALA:HB2	1.94	0.48
2:B:7:ALA:HA	2:B:39:ARG:O	2.13	0.48
2:B:124:GLY:O	2:B:127:ARG:HG3	2.13	0.48
2:A:267:ARG:HD3	6:A:1033:HOH:O	2.12	0.47
2:A:6:ILE:C	2:A:8:PRO:HD3	2.35	0.47
2:A:347:TYR:CE1	2:A:453:LEU:HD22	2.49	0.47
1:C:569:G:O2'	1:C:570:G:H5'	2.14	0.47
2:B:73:VAL:O	2:B:73:VAL:HG12	2.12	0.47
2:A:422:GLU:HG3	2:A:423:LYS:N	2.28	0.47
2:A:116:ARG:HA	2:A:121:GLY:H	1.79	0.47
2:B:409:GLU:HG3	6:B:1032:HOH:O	2.13	0.47
2:B:81:ARG:HB2	2:B:84:GLU:HG3	1.95	0.47
2:B:6:ILE:HD12	2:B:21:ILE:HG22	1.96	0.47
2:B:37:ILE:CG2	2:B:38:VAL:N	2.76	0.47
2:A:163:ARG:NH1	2:A:300:LEU:CD1	2.73	0.47
2:A:444:THR:HB	2:A:445:PRO:HD2	1.96	0.47
2:A:110:GLU:H	2:A:110:GLU:CD	2.16	0.47
2:B:296:GLU:OE1	2:B:296:GLU:N	2.48	0.47
2:A:439:THR:HG21	2:A:444:THR:HG21	1.97	0.47
2:A:283:ILE:HD13	2:A:313:MET:CE	2.44	0.47
2:B:86:LEU:HD21	2:B:184:TYR:CE1	2.50	0.47
2:A:268:ASN:C	2:A:268:ASN:HD22	2.19	0.47
2:A:257:LYS:HE3	6:A:1019:HOH:O	2.14	0.46
2:B:241:LYS:HE2	2:B:304:VAL:HG21	1.96	0.46
2:B:133:GLU:O	2:B:137:ARG:HG3	2.16	0.46
2:B:106:PHE:CD2	2:B:144:HIS:HB3	2.51	0.46
2:A:96:LEU:HD13	2:A:223:PHE:CE1	2.49	0.46
2:B:435:ARG:NH1	2:B:444:THR:CG2	2.71	0.46
2:B:45:ARG:HD3	2:B:184:TYR:CZ	2.51	0.46
2:B:85:ARG:NH1	2:B:194:ASP:OD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:ASP:HB3	2:A:200:VAL:HG22	1.98	0.46
2:B:391:LEU:N	2:B:392:PRO:CD	2.79	0.46
2:A:170:ASN:HA	2:A:173:ILE:HD12	1.98	0.46
2:A:37:ILE:HG22	2:A:38:VAL:N	2.30	0.45
2:A:53:GLU:O	2:A:56:ILE:HG22	2.16	0.45
2:A:330:ARG:O	2:A:362:LEU:HD13	2.16	0.45
2:B:391:LEU:O	2:B:395:LYS:HG3	2.17	0.45
1:D:508:U:C2	1:D:515:G:O6	2.70	0.45
2:B:179:LEU:HD21	2:B:183:GLY:O	2.15	0.45
2:B:369:ALA:HB1	2:B:372:LEU:HD12	1.98	0.45
2:B:98:LYS:HD2	2:B:98:LYS:N	2.30	0.45
2:B:176:VAL:HG11	2:B:215:ILE:HD13	1.98	0.45
1:C:575:C:H2'	1:C:576:A:O4'	2.16	0.45
2:A:294:THR:CG2	2:A:296:GLU:HB2	2.46	0.45
1:C:571:U:H2'	1:C:572:C:C6	2.52	0.45
2:B:115:ILE:HD13	2:B:116:ARG:N	2.32	0.45
2:A:294:THR:HG23	2:A:296:GLU:OE1	2.16	0.45
1:C:534:C:O2	2:A:435:ARG:NH2	2.39	0.45
1:D:552:G:H5'	1:D:553:G:OP2	2.17	0.44
2:B:463:LEU:O	2:B:467:LEU:HG	2.17	0.44
2:B:417:ARG:HG2	2:B:417:ARG:HH11	1.82	0.44
2:A:294:THR:CG2	2:A:296:GLU:H	2.29	0.44
2:A:133:GLU:O	2:A:137:ARG:HG3	2.17	0.44
2:B:205:ARG:HD3	2:B:232:HIS:CD2	2.52	0.44
2:B:286:LEU:O	2:B:290:ILE:HG23	2.18	0.44
2:B:30:ARG:HD3	6:B:1014:HOH:O	2.17	0.44
2:A:203:VAL:HA	6:A:1039:HOH:O	2.16	0.44
2:B:179:LEU:HD21	2:B:183:GLY:C	2.38	0.44
2:B:239:PRO:HA	2:B:304:VAL:HG13	1.98	0.44
2:B:324:LEU:HD23	2:B:324:LEU:O	2.18	0.44
2:B:350:ARG:HG3	2:B:453:LEU:HD13	2.00	0.44
2:A:136:GLU:OE2	2:A:139:ARG:NH1	2.51	0.44
2:B:86:LEU:HB2	2:B:87:PRO:HD3	2.00	0.44
2:A:310:LEU:O	2:A:310:LEU:HD22	2.17	0.43
2:A:404:GLN:HG3	2:A:415:LEU:HD22	2.00	0.43
2:B:79:PRO:HB3	2:B:84:GLU:OE1	2.18	0.43
2:A:1:MET:HE3	2:A:2:VAL:O	2.18	0.43
1:D:549:G:N2	1:D:566:U:H1'	2.34	0.43
2:A:404:GLN:HE21	2:A:415:LEU:HD13	1.84	0.43
2:A:176:VAL:HG11	2:A:215:ILE:HD13	2.01	0.43
1:C:525:C:H5''	2:A:312:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:THR:N	2:B:214:PRO:CD	2.81	0.43
1:D:506:C:C2'	1:D:507:A:H5'	2.48	0.43
2:B:423:LYS:NZ	2:B:423:LYS:CB	2.82	0.43
2:A:454:LEU:HB3	2:A:458:ARG:HD2	2.00	0.43
2:A:106:PHE:CD2	2:A:144:HIS:HB3	2.54	0.43
2:A:15:HIS:O	2:A:18:THR:HB	2.18	0.43
2:A:404:GLN:NE2	2:A:415:LEU:HD13	2.34	0.43
2:A:332:LYS:HB2	2:A:333:PRO:HD3	2.01	0.42
2:B:237:ARG:HH11	2:B:302:GLY:HA3	1.83	0.42
2:A:105:ALA:HB1	2:A:107:GLU:OE2	2.19	0.42
2:B:446:GLY:O	2:B:449:GLU:HG2	2.19	0.42
1:C:536:C:H2'	1:C:537:A:O4'	2.19	0.42
2:B:425:VAL:HG22	2:B:429:GLN:NE2	2.34	0.42
1:D:576:A:H3'	2:B:187:TYR:CD1	2.55	0.42
2:A:150:VAL:HA	2:A:151:PRO:HD3	1.87	0.42
1:D:501:G:H2'	1:D:502:G:C8	2.55	0.42
2:B:463:LEU:HD22	2:B:467:LEU:HD11	2.00	0.42
2:A:211:VAL:HG22	6:A:1049:HOH:O	2.19	0.42
2:B:122:TYR:CE2	2:B:124:GLY:HA2	2.55	0.42
2:B:10:PRO:CB	2:B:52:ALA:HB3	2.50	0.42
2:B:131:PRO:O	2:B:135:GLU:HG2	2.20	0.42
2:B:6:ILE:HD13	2:B:21:ILE:HG22	2.02	0.42
2:A:19:ALA:HB1	2:A:63:LEU:CD1	2.50	0.42
1:C:508:U:C2	1:C:515:G:O6	2.73	0.42
2:A:460:LEU:O	2:A:464:GLU:HG3	2.20	0.42
2:A:7:ALA:HB1	2:A:41:GLU:HG3	2.02	0.41
2:A:10:PRO:HG3	2:A:42:ASP:HB3	2.01	0.41
2:B:116:ARG:CD	2:B:121:GLY:H	2.33	0.41
2:B:206:ALA:HB3	5:B:602:GSU:O2'	2.19	0.41
1:C:521:A:H61	1:C:546:A:H2'	1.85	0.41
1:C:543:G:H2'	1:C:544:A:C8	2.55	0.41
2:A:119:LYS:HD2	2:A:123:ASP:OD2	2.19	0.41
1:C:574:C:C4'	2:A:177:VAL:HG21	2.51	0.41
2:B:290:ILE:CD1	2:B:290:ILE:C	2.87	0.41
2:B:127:ARG:HH21	2:B:175:ASP:CG	2.23	0.41
2:B:117:LYS:HB2	2:B:117:LYS:NZ	2.36	0.41
2:B:14:PRO:HB3	2:B:56:ILE:HA	2.00	0.41
2:B:267:ARG:HD2	2:B:286:LEU:HD13	2.02	0.41
1:D:536:C:H2'	1:D:537:A:O4'	2.21	0.41
2:B:450:ILE:HA	2:B:450:ILE:HD13	1.84	0.41
2:B:255:TRP:CZ2	2:B:259:GLU:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:THR:CG2	2:B:294:THR:O	2.68	0.41
2:B:402:ARG:HH11	2:B:402:ARG:CG	2.34	0.41
2:B:107:GLU:N	2:B:107:GLU:OE2	2.34	0.41
2:B:445:PRO:HG2	2:B:450:ILE:CG1	2.51	0.41
2:A:445:PRO:HG2	2:A:450:ILE:CD1	2.50	0.41
2:B:82:GLN:HG2	2:B:194:ASP:OD1	2.21	0.41
1:D:514:A:C2'	1:D:515:G:H5'	2.51	0.41
2:B:140:ARG:HA	2:B:140:ARG:NE	2.35	0.41
2:A:102:ALA:HB1	2:A:147:ARG:O	2.20	0.41
2:B:393:LEU:HD13	2:B:430:VAL:HG22	2.02	0.41
2:B:20:TYR:OH	2:B:234:PRO:HD2	2.21	0.41
2:B:88:LEU:HD21	2:B:197:LEU:CD1	2.51	0.41
2:B:262:LEU:HD22	2:B:330:ARG:HH11	1.86	0.40
2:B:78:GLY:HA2	2:B:79:PRO:O	2.20	0.40
2:A:31:ARG:O	2:A:31:ARG:HG3	2.21	0.40
2:A:239:PRO:HA	2:A:304:VAL:HG13	2.02	0.40
2:B:92:TYR:O	2:B:95:GLU:HB3	2.21	0.40
2:B:354:LEU:HD22	2:B:449:GLU:HG3	2.02	0.40
2:A:335:LEU:HD23	2:A:335:LEU:HA	1.89	0.40
1:C:504:C:H2'	1:C:505:C:H6	1.86	0.40
2:B:290:ILE:O	2:B:290:ILE:HD12	2.20	0.40
1:D:565:C:O2'	1:D:566:U:H5'	2.22	0.40
2:B:386:LYS:HE2	2:B:432:GLN:CG	2.49	0.40
2:B:174:PRO:HG2	2:B:176:VAL:CG1	2.52	0.40
2:B:113:GLU:HA	2:B:113:GLU:OE1	2.20	0.40
2:B:152:ARG:HH11	2:B:152:ARG:HG2	1.86	0.40
2:B:274:GLY:O	2:B:298:VAL:HA	2.22	0.40
2:B:1:MET:HB2	2:B:2:VAL:H	1.65	0.40
2:B:383:ALA:HA	2:B:442:LEU:HD13	2.04	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:A:343:GLU:O	2:B:50:PRO:O[6_654]	2.16	0.04

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	
2	A	466/468 (100%)	453 (97%)	12 (3%)	1 (0%)	52	80
2	B	466/468 (100%)	448 (96%)	16 (3%)	2 (0%)	39	69
All	All	932/936 (100%)	901 (97%)	28 (3%)	3 (0%)	46	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	GLY
2	B	120	GLY
2	B	151	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	
2	A	393/393 (100%)	366 (93%)	27 (7%)	19	43
2	B	393/393 (100%)	356 (91%)	37 (9%)	11	25
All	All	786/786 (100%)	722 (92%)	64 (8%)	15	33

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	ARG
2	A	67	TYR
2	A	96	LEU

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Mol	Chain	Res	Type
2	A	97	LEU
2	A	132	GLU
2	A	185	PRO
2	A	189	LEU
2	A	197	LEU
2	A	200	VAL
2	A	205	ARG
2	A	218	LEU
2	A	236	LEU
2	A	247	ARG
2	A	268	ASN
2	A	270	LEU
2	A	272	LEU
2	A	286	LEU
2	A	294	THR
2	A	310	LEU
2	A	343	GLU
2	A	356	ARG
2	A	391	LEU
2	A	442	LEU
2	A	453	LEU
2	A	454	LEU
2	A	457	GLU
2	A	458	ARG
2	B	1	MET
2	B	5	ARG
2	B	21	ILE
2	B	86	LEU
2	B	90	GLN
2	B	115	ILE
2	B	116	ARG
2	B	119	LYS
2	B	123	ASP
2	B	128	ASN
2	B	179	LEU
2	B	189	LEU
2	B	205	ARG
2	B	218	LEU
2	B	236	LEU
2	B	259	GLU
2	B	266	LEU
2	B	268	ASN

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Mol	Chain	Res	Type
2	B	270	LEU
2	B	272	LEU
2	B	290	ILE
2	B	310	LEU
2	B	324	LEU
2	B	326	GLU
2	B	355	MET
2	B	356	ARG
2	B	405	GLU
2	B	406	GLU
2	B	412	LEU
2	B	423	LYS
2	B	425	VAL
2	B	432	GLN
2	B	442	LEU
2	B	444	THR
2	B	449	GLU
2	B	454	LEU
2	B	463	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	90	GLN
2	A	114	GLN
2	A	404	GLN
2	A	429	GLN
2	B	25	ASN
2	B	90	GLN
2	B	191	ASN
2	B	404	GLN
2	B	432	GLN

5.3.3   RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	14 (18%)	6 (8%)
1	D	74/75 (98%)	13 (17%)	6 (8%)
All	All	148/150 (98%)	27 (18%)	12 (8%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U
1	C	509	C
1	C	516	C
1	C	518	G
1	C	519	G
1	C	520	U
1	C	548	C
1	C	553	G
1	C	558	A
1	C	559	U
1	C	573	A
1	C	574	C
1	C	575	C
1	D	508	U
1	D	509	C
1	D	516	C
1	D	518	G
1	D	519	G
1	D	520	U
1	D	548	C
1	D	553	G
1	D	558	A
1	D	559	U
1	D	573	A
1	D	574	C
1	D	575	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	509	C
1	C	518	G
1	C	519	G
1	C	558	A
1	C	573	A
1	D	507	A
1	D	518	G
1	D	519	G
1	D	558	A
1	D	560	U

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Mol	Chain	Res	Type
1	D	573	A

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 carbohydrates 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	#$|Z| > 2$
5	GSU	A	601	-	24,34,34	1.78	4 (16%)	30,50,50	2.02	3 (10%)
5	GSU	B	602	-	24,34,34	1.35	2 (8%)	30,50,50	1.95	6 (20%)

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
5	GSU	A	601	-	-	0/16/40/40	0/3/3/3
5	GSU	B	602	-	-	0/16/40/40	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	GSU	O4'-C1'	2.04	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	GSU	C2-N3	2.41	1.36	1.32
5	B	602	GSU	O2S-S	2.51	1.44	1.42
5	B	602	GSU	O1S-S	4.56	1.46	1.42
5	A	601	GSU	O1S-S	4.57	1.46	1.42
5	A	601	GSU	O2S-S	5.71	1.47	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	GSU	O2S-S-O1S	-8.02	111.16	120.77
5	B	602	GSU	O2S-S-O1S	-7.49	111.80	120.77
5	A	601	GSU	CB-CA-N	-3.43	102.62	109.81
5	B	602	GSU	CB-CA-N	-2.21	105.17	109.81
5	B	602	GSU	C4-C5-N7	2.12	111.43	109.48
5	B	602	GSU	O-C-CA	2.22	125.37	119.80
5	B	602	GSU	O4'-C1'-N9	2.64	113.63	108.10
5	B	602	GSU	O5'-C5'-C4'	4.22	116.01	107.90
5	A	601	GSU	O5'-C5'-C4'	4.55	116.65	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	GSU	2	0
5	B	602	GSU	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	75/75 (100%)	-0.16	2 (2%)	58	58	25, 43, 76, 83	0
1	D	75/75 (100%)	-0.14	2 (2%)	58	58	21, 41, 75, 96	0
2	A	468/468 (100%)	-0.29	5 (1%)	82	83	13, 29, 61, 75	0
2	B	468/468 (100%)	-0.18	11 (2%)	62	62	13, 32, 76, 95	0
All	All	1086/1086 (100%)	-0.22	20 (1%)	71	72	13, 32, 70, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	ASN	5.4
1	D	516	C	4.6
2	B	140	ARG	4.0
2	A	468	ALA	3.5
2	B	141	GLY	3.3
2	B	133	GLU	3.1
2	B	139	ARG	2.9
2	A	401	LEU	2.8
2	B	1	MET	2.8
2	A	1	MET	2.7
2	B	118	GLU	2.5
2	B	136	GLU	2.5
2	A	376	ASP	2.5
1	C	516	C	2.3
2	B	132	GLU	2.3
2	B	130	PRO	2.2
1	C	558	A	2.2
2	B	129	ILE	2.2
2	A	405	GLU	2.1
1	D	558	A	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	CL	A	904	1/1	0.99	0.30	3.93	33,33,33,33	0
5	GSU	A	601	32/32	0.98	0.14	-0.65	16,22,28,31	0
5	GSU	B	602	32/32	0.98	0.14	-1.08	16,25,31,32	0
3	MG	D	901	1/1	0.94	0.27	-	33,33,33,33	0
3	MG	C	902	1/1	0.88	0.20	-	36,36,36,36	0
4	CL	B	903	1/1	0.98	0.25	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.