



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:06 pm BST

PDB ID : 2ALY  
Title : Crystal Structure of T.Thermophilus Phenylalanyl-tRNA synthetase complexed with 5'-O-[N-(L-tyrosyl)sulphamoyl]adenosine  
Authors : Kotik-Kogan, O.M.; Moor, N.A.; Tworowski, D.E.; Safro, M.G.  
Deposited on : 2005-08-04  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

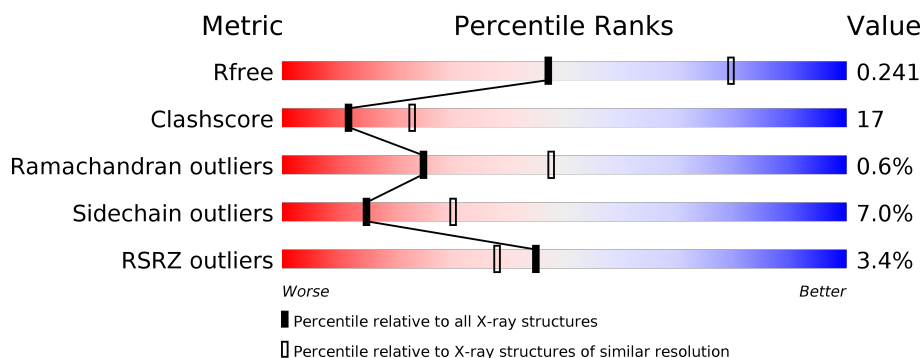
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>.</div> </div> </div>
2	B	785	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>



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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2123	1388	363	365	7			

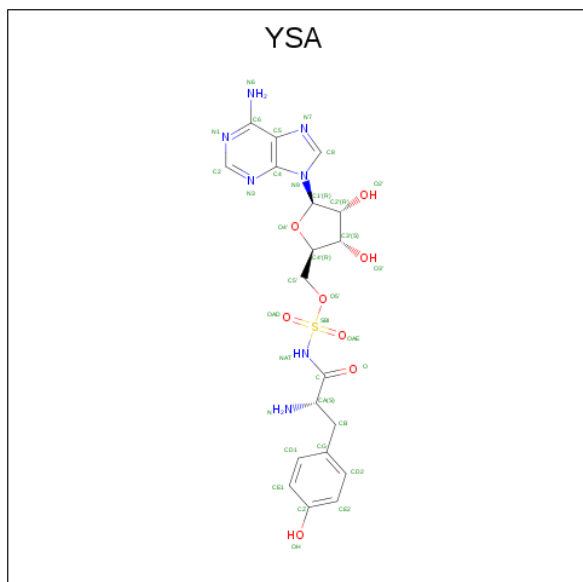
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0

- Molecule 4 is 5'-O-[N-(L-TYROSYL)SULFAMOYL]ADENOSINE (three-letter code: YSA) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>7</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			35	19	7	8	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

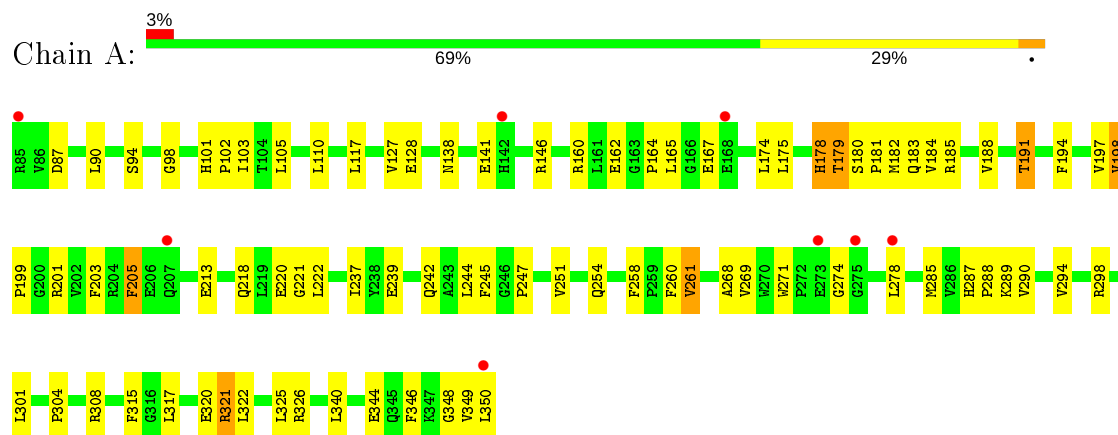
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	B	173	Total	O	0	0
			173	173		

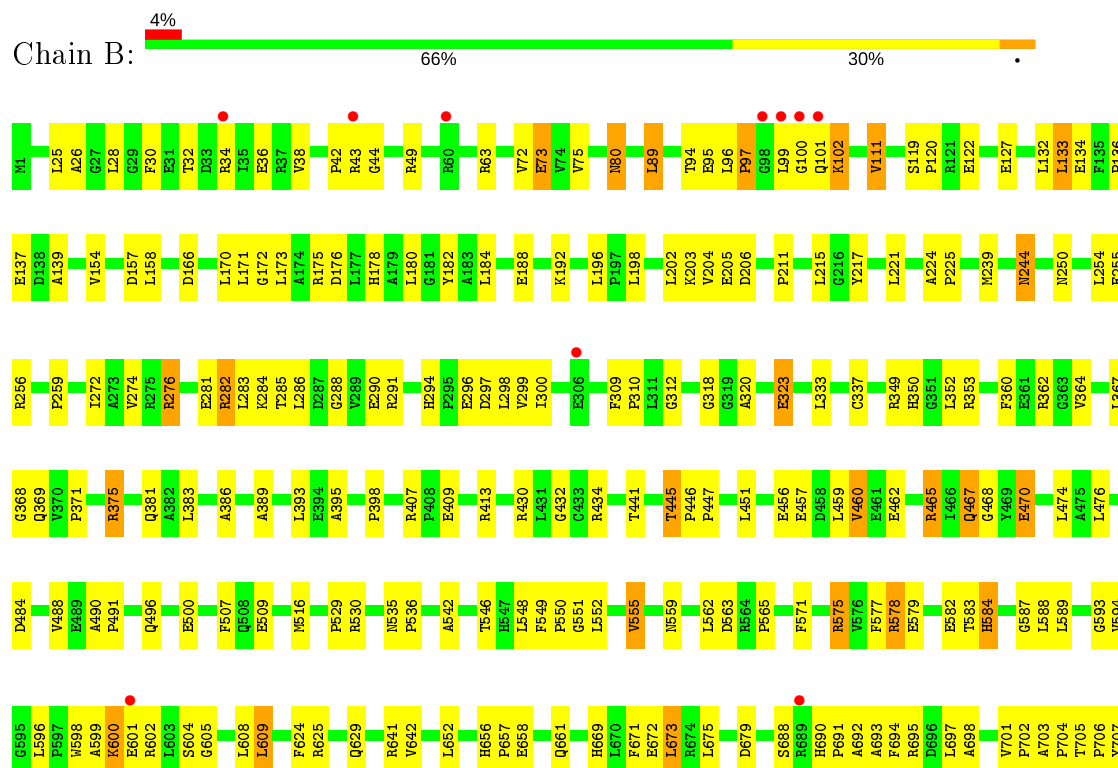
### 3 Residue-property plots

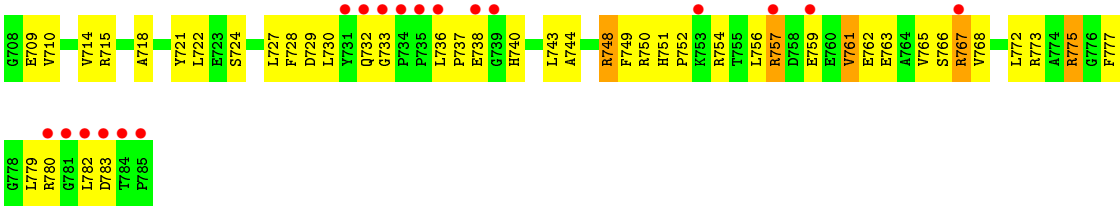
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Phenylalanyl-tRNA synthetase alpha chain



- Molecule 2: Phenylalanyl-tRNA synthetase beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.64Å 173.64Å 139.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.59 – 2.60 24.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.59-2.60) 100.0 (24.59-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.246 0.221 , 0.241	Depositor DCC
$R_{free}$ test set	3757 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YSA, MN, SO4

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	0.43	0/2191	0.64	0/2971
2	B	0.38	0/6280	0.66	2/8536 (0.0%)
All	All	0.40	0/8471	0.66	2/11507 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	6.56	128.72	111.00
2	B	133	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2123	0	2075	71	0
2	B	6127	0	6180	228	1
3	A	1	0	0	0	0
4	A	35	0	22	2	0
5	B	5	0	0	0	0
6	A	58	0	0	3	0
6	B	173	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8522	0	8277	289	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 17.

All (289) 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:B:192:LYS:H	2:B:381:GLN:HE22	1.07	0.99
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.32	0.93
2:B:286:LEU:HD22	2:B:323:GLU:HG2	1.52	0.91
1:A:278:LEU:HD13	1:A:325:LEU:HD22	1.52	0.90
2:B:286:LEU:CD2	2:B:323:GLU:HG2	2.03	0.88
1:A:191:THR:HG22	2:B:484:ASP:OD2	1.75	0.85
2:B:286:LEU:HD23	2:B:320:ALA:HA	1.57	0.85
2:B:600:LYS:HD3	2:B:600:LYS:N	1.94	0.82
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.63	0.81
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.45	0.80
2:B:762:GLU:O	2:B:765:VAL:HG22	1.83	0.79
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.65	0.78
2:B:600:LYS:HD3	2:B:600:LYS:H	1.48	0.78
2:B:80:ASN:H	2:B:80:ASN:HD22	1.29	0.78
2:B:101:GLN:HA	2:B:101:GLN:HE21	1.48	0.76
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.51	0.76
2:B:516:MET:SD	2:B:529:PRO:HG3	2.26	0.75
2:B:80:ASN:HD21	2:B:132:LEU:H	1.31	0.75
2:B:99:LEU:HD12	2:B:101:GLN:H	1.51	0.74
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.71	0.72
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.90	0.72
2:B:516:MET:HE3	2:B:546:THR:H	1.55	0.72
2:B:192:LYS:N	2:B:381:GLN:HE22	1.86	0.71
1:A:183:GLN:HG3	1:A:222:LEU:HD22	1.72	0.71
2:B:409:GLU:OE2	2:B:413:ARG:NH1	2.23	0.71
2:B:496:GLN:O	2:B:500:GLU:HG3	1.91	0.71
2:B:575:ARG:HH11	2:B:575:ARG:HG2	1.55	0.71
1:A:244:LEU:HD21	1:A:322:LEU:HD21	1.71	0.70
2:B:239:MET:HE2	2:B:254:LEU:HD11	1.73	0.70
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.74	0.70
1:A:242:GLN:OE1	1:A:247:PRO:HA	1.91	0.69
2:B:198:LEU:HD13	2:B:217:TYR:HB2	1.73	0.69
2:B:751:HIS:HB3	2:B:754:ARG:O	1.93	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.94	0.67
2:B:407:ARG:HD3	2:B:456:GLU:OE2	1.94	0.67
2:B:551:GLY:O	2:B:555:VAL:HG12	1.93	0.67
1:A:278:LEU:HD13	1:A:325:LEU:CD2	2.25	0.66
2:B:730:LEU:HD13	2:B:743:LEU:HD23	1.77	0.66
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.25	0.66
2:B:767:ARG:N	2:B:767:ARG:HE	1.94	0.65
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.06	0.65
1:A:160:ARG:NH2	2:B:579:GLU:HB3	2.12	0.65
2:B:101:GLN:HA	2:B:101:GLN:NE2	2.12	0.64
2:B:178:HIS:O	2:B:430:ARG:NH1	2.31	0.64
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.80	0.63
2:B:467:GLN:NE2	2:B:467:GLN:HA	2.14	0.63
2:B:323:GLU:HA	2:B:323:GLU:OE2	1.99	0.62
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.34	0.62
2:B:578:ARG:O	2:B:579:GLU:HB2	1.99	0.62
2:B:761:VAL:O	2:B:765:VAL:HG13	1.99	0.62
2:B:291:ARG:NH2	2:B:352:LEU:HD21	2.15	0.62
1:A:340:LEU:O	1:A:344:GLU:HG3	2.00	0.61
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.65	0.61
2:B:763:GLU:OE2	2:B:767:ARG:HD2	1.99	0.61
2:B:80:ASN:N	2:B:80:ASN:HD22	1.98	0.61
2:B:96:LEU:HD12	2:B:99:LEU:HD21	1.83	0.61
2:B:224:ALA:H	2:B:244:ASN:ND2	1.99	0.61
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.84	0.60
1:A:110:LEU:HD21	1:A:322:LEU:CD2	2.31	0.60
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.83	0.60
1:A:237:ILE:HG22	1:A:251:VAL:HG11	1.83	0.60
2:B:285:THR:O	2:B:320:ALA:HB2	2.02	0.60
2:B:467:GLN:HE21	2:B:467:GLN:CA	2.11	0.60
2:B:702:PRO:C	2:B:704:PRO:HD2	2.23	0.59
2:B:737:PRO:O	2:B:738:GLU:C	2.38	0.59
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.37	0.58
2:B:239:MET:HE1	2:B:250:ASN:HB3	1.85	0.58
2:B:730:LEU:HD13	2:B:743:LEU:CD2	2.33	0.58
2:B:99:LEU:O	2:B:101:GLN:N	2.37	0.58
2:B:286:LEU:HD21	2:B:323:GLU:HG2	1.83	0.58
2:B:588:LEU:HD23	2:B:588:LEU:C	2.24	0.57
2:B:224:ALA:N	2:B:244:ASN:HD22	2.02	0.57
2:B:462:GLU:OE1	2:B:465:ARG:NH1	2.35	0.57
1:A:110:LEU:HD21	1:A:322:LEU:HD23	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.69	0.57
2:B:575:ARG:NH1	2:B:575:ARG:HG2	2.19	0.57
1:A:160:ARG:HH21	2:B:579:GLU:HB3	1.70	0.56
1:A:184:VAL:O	1:A:188:VAL:HG13	2.05	0.56
1:A:141:GLU:HG2	1:A:146:ARG:NH1	2.20	0.56
2:B:701:VAL:CG1	2:B:705:THR:HB	2.34	0.56
1:A:180:SER:O	1:A:183:GLN:HB3	2.05	0.56
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.19	0.56
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.88	0.56
1:A:138:ASN:OD1	1:A:289:LYS:HE3	2.06	0.56
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.88	0.55
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.41	0.55
2:B:224:ALA:N	2:B:244:ASN:ND2	2.54	0.55
2:B:224:ALA:H	2:B:244:ASN:HD22	1.53	0.55
2:B:294:HIS:HB2	2:B:349:ARG:HD3	1.89	0.55
1:A:350:LEU:HD22	1:A:350:LEU:N	2.22	0.55
2:B:432:GLY:C	2:B:447:PRO:HG3	2.27	0.55
2:B:297:ASP:OD2	2:B:350:HIS:HE1	1.90	0.55
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.88	0.55
2:B:604:SER:HA	2:B:608:LEU:HD22	1.87	0.55
2:B:43:ARG:HH11	2:B:43:ARG:HG3	1.72	0.54
2:B:282:ARG:NH1	2:B:290:GLU:HG3	2.22	0.54
2:B:274:VAL:CG1	2:B:298:LEU:HD11	2.37	0.54
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.41	0.54
2:B:768:VAL:O	2:B:772:LEU:HB2	2.07	0.54
2:B:178:HIS:HD2	2:B:182:TYR:O	1.90	0.54
2:B:703:ALA:N	2:B:704:PRO:HD2	2.23	0.53
2:B:701:VAL:HG13	2:B:777:PHE:CE1	2.43	0.53
2:B:629:GLN:OE1	2:B:641:ARG:HD3	2.07	0.53
2:B:353:ARG:C	2:B:353:ARG:HD3	2.29	0.53
2:B:732:GLN:HG3	2:B:732:GLN:O	2.07	0.53
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.43	0.53
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.90	0.53
2:B:782:LEU:HD23	2:B:783:ASP:N	2.24	0.53
2:B:198:LEU:N	2:B:198:LEU:HD23	2.23	0.53
2:B:367:LEU:HD21	2:B:398:PRO:HB2	1.91	0.53
1:A:258:PHE:CE2	4:A:999:YSA:HD1	2.43	0.53
1:A:317:LEU:C	1:A:317:LEU:HD12	2.30	0.53
2:B:432:GLY:O	2:B:447:PRO:HG3	2.08	0.53
2:B:690:HIS:HB3	2:B:691:PRO:HD2	1.91	0.53
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.92	0.52
1:A:101:HIS:CE1	1:A:103:ILE:HG12	2.44	0.52
2:B:657:PRO:O	2:B:661:GLN:OE1	2.28	0.52
2:B:672:GLU:C	2:B:673:LEU:HD23	2.30	0.52
2:B:284:LYS:HZ1	2:B:288:GLY:HA2	1.75	0.52
2:B:368:GLY:O	2:B:371:PRO:HD2	2.10	0.52
2:B:759:GLU:O	2:B:763:GLU:HB2	2.10	0.52
2:B:698:ALA:O	2:B:779:LEU:HD12	2.10	0.52
2:B:299:VAL:HG11	2:B:310:PRO:HB3	1.91	0.52
2:B:101:GLN:O	2:B:102:LYS:C	2.48	0.52
2:B:34:ARG:HH11	2:B:34:ARG:HG2	1.75	0.52
2:B:692:ALA:HB2	2:B:750:ARG:HD2	1.92	0.52
2:B:697:LEU:O	2:B:697:LEU:HD12	2.10	0.52
2:B:733:GLY:O	2:B:736:LEU:HB2	2.10	0.52
2:B:763:GLU:O	2:B:767:ARG:HG2	2.10	0.52
1:A:174:LEU:HD12	1:A:174:LEU:C	2.30	0.51
2:B:693:ALA:O	2:B:748:ARG:HA	2.10	0.51
2:B:42:PRO:HG2	2:B:95:GLU:O	2.10	0.51
2:B:721:TYR:O	2:B:749:PHE:HA	2.10	0.51
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.41	0.50
1:A:205:PHE:HD2	2:B:535:ASN:HD22	1.59	0.50
2:B:434:ARG:HB3	2:B:445:THR:HG23	1.93	0.50
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.14	0.50
2:B:284:LYS:NZ	2:B:288:GLY:HA2	2.26	0.50
1:A:128:GLU:OE1	1:A:185:ARG:NH1	2.45	0.50
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.47	0.50
1:A:102:PRO:HG3	1:A:346:PHE:CD1	2.47	0.50
2:B:462:GLU:CD	2:B:465:ARG:NH1	2.65	0.50
2:B:600:LYS:HG2	2:B:601:GLU:OE2	2.12	0.49
1:A:101:HIS:ND1	1:A:102:PRO:HD2	2.26	0.49
1:A:162:GLU:O	1:A:185:ARG:NH2	2.45	0.49
2:B:99:LEU:HD12	2:B:101:GLN:N	2.23	0.49
2:B:757:ARG:HG2	2:B:757:ARG:HH11	1.78	0.49
2:B:530:ARG:HD2	2:B:579:GLU:H	1.77	0.49
2:B:368:GLY:C	2:B:371:PRO:HD2	2.33	0.49
2:B:552:LEU:HA	2:B:555:VAL:HG13	1.95	0.49
2:B:192:LYS:H	2:B:381:GLN:NE2	1.91	0.49
2:B:221:LEU:HD23	2:B:386:ALA:HB2	1.94	0.49
2:B:202:LEU:HB2	2:B:393:LEU:HD23	1.95	0.49
1:A:348:GLY:O	1:A:350:LEU:N	2.46	0.49
2:B:697:LEU:HD12	2:B:697:LEU:C	2.33	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:LEU:O	2:B:555:VAL:HG13	2.13	0.48
2:B:563:ASP:C	2:B:565:PRO:HD3	2.34	0.48
2:B:695:ARG:CZ	2:B:761:VAL:HG11	2.43	0.48
1:A:205:PHE:HD2	2:B:535:ASN:ND2	2.12	0.48
2:B:549:PHE:CD2	2:B:550:PRO:HD3	2.49	0.48
1:A:117:LEU:HD21	1:A:239:GLU:HG3	1.96	0.48
2:B:217:TYR:HD2	2:B:389:ALA:HB2	1.78	0.48
2:B:656:HIS:HE1	2:B:658:GLU:HG3	1.79	0.48
1:A:317:LEU:O	1:A:317:LEU:HD12	2.12	0.47
2:B:239:MET:CE	2:B:250:ASN:HB3	2.43	0.47
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.28	0.47
2:B:552:LEU:HA	2:B:555:VAL:CG1	2.44	0.47
2:B:584:HIS:HD2	2:B:672:GLU:OE2	1.96	0.47
2:B:134:GLU:O	2:B:225:PRO:HB3	2.15	0.47
2:B:239:MET:HE2	2:B:254:LEU:CD1	2.41	0.47
2:B:281:GLU:HG2	2:B:310:PRO:HG2	1.96	0.47
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.30	0.47
2:B:286:LEU:HG	2:B:318:GLY:O	2.15	0.47
2:B:710:VAL:O	2:B:714:VAL:HG23	2.15	0.47
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.50	0.47
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.97	0.47
2:B:203:LYS:HE3	2:B:205:GLU:OE2	2.15	0.47
2:B:299:VAL:HG13	2:B:312:GLY:O	2.14	0.47
2:B:688:SER:HB2	2:B:752:PRO:HA	1.97	0.47
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.44	0.47
2:B:99:LEU:C	2:B:101:GLN:H	2.18	0.47
2:B:36:GLU:O	2:B:154:VAL:HA	2.15	0.47
2:B:698:ALA:HB3	2:B:780:ARG:HB3	1.95	0.47
2:B:714:VAL:O	2:B:718:ALA:HB2	2.15	0.47
2:B:96:LEU:HB2	2:B:99:LEU:HG	1.96	0.47
2:B:609:LEU:HD13	2:B:652:LEU:HD11	1.97	0.47
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.15	0.46
1:A:141:GLU:HA	1:A:146:ARG:HG3	1.97	0.46
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.97	0.46
2:B:274:VAL:HG12	2:B:298:LEU:HD11	1.96	0.46
2:B:724:SER:HB2	2:B:748:ARG:HD3	1.96	0.46
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.96	0.46
2:B:718:ALA:HB3	2:B:722:LEU:HD22	1.97	0.46
1:A:258:PHE:CZ	4:A:999:YSA:HD1	2.51	0.46
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.80	0.46
2:B:34:ARG:NH1	2:B:157:ASP:OD2	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:GLU:HG3	2:B:188:GLU:O	2.16	0.46
2:B:596:LEU:HB2	2:B:599:ALA:CB	2.45	0.46
2:B:602:ARG:NH1	2:B:602:ARG:CG	2.75	0.46
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.46	0.45
2:B:80:ASN:H	2:B:80:ASN:ND2	2.07	0.45
2:B:49:ARG:CD	2:B:137:GLU:HG3	2.47	0.45
2:B:707:TYR:CE1	2:B:727:LEU:HD22	2.52	0.45
2:B:530:ARG:HH11	2:B:530:ARG:HB2	1.82	0.45
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.98	0.45
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.51	0.45
2:B:299:VAL:HG12	2:B:300:ILE:N	2.31	0.45
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.98	0.45
1:A:254:GLN:NE2	2:B:26:ALA:HB1	2.31	0.45
2:B:451:LEU:N	2:B:451:LEU:HD23	2.32	0.45
2:B:549:PHE:O	2:B:550:PRO:C	2.55	0.45
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.52	0.45
2:B:766:SER:HB3	2:B:767:ARG:HH21	1.82	0.45
2:B:175:ARG:O	2:B:178:HIS:HB3	2.17	0.45
2:B:323:GLU:CA	2:B:323:GLU:OE2	2.64	0.45
2:B:457:GLU:O	2:B:460:VAL:HG13	2.17	0.44
6:A:1014:HOH:O	2:B:476:LEU:HD23	2.17	0.44
1:A:98:GLY:HA3	2:B:507:PHE:O	2.17	0.44
2:B:718:ALA:O	2:B:749:PHE:HE2	2.01	0.44
2:B:136:PRO:HD2	2:B:139:ALA:HB2	1.99	0.44
1:A:191:THR:CG2	2:B:484:ASP:OD2	2.56	0.44
2:B:604:SER:HA	2:B:608:LEU:HB2	2.00	0.44
2:B:695:ARG:NH1	2:B:761:VAL:HG11	2.32	0.44
2:B:43:ARG:NH1	2:B:43:ARG:HG3	2.31	0.44
2:B:119:SER:OG	2:B:122:GLU:HG3	2.18	0.44
2:B:457:GLU:HA	2:B:460:VAL:CG1	2.48	0.44
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.32	0.44
2:B:367:LEU:CD2	2:B:398:PRO:HB2	2.47	0.43
1:A:164:PRO:HD2	1:A:167:GLU:OE2	2.19	0.43
1:A:94:SER:O	2:B:594:VAL:HG13	2.17	0.43
2:B:369:GLN:CD	2:B:369:GLN:H	2.21	0.43
2:B:715:ARG:NH1	2:B:715:ARG:HB2	2.33	0.43
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.54	0.43
2:B:555:VAL:HG23	2:B:559:ASN:HD22	1.84	0.43
2:B:773:ARG:HG2	2:B:777:PHE:O	2.17	0.43
2:B:694:PHE:CD1	2:B:694:PHE:N	2.87	0.43
1:A:268:ALA:HA	1:A:278:LEU:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:HG21	2:B:395:ALA:HB3	2.01	0.43
1:A:101:HIS:HE1	1:A:103:ILE:HG12	1.84	0.43
2:B:99:LEU:O	2:B:101:GLN:HG2	2.18	0.43
1:A:298:ARG:NH1	1:A:304:PRO:O	2.48	0.42
1:A:164:PRO:HG2	1:A:188:VAL:HG21	2.02	0.42
2:B:192:LYS:O	2:B:192:LYS:HD3	2.18	0.42
2:B:600:LYS:HG2	2:B:601:GLU:CD	2.40	0.42
2:B:729:ASP:HB3	2:B:744:ALA:HB3	2.02	0.42
2:B:757:ARG:HA	2:B:757:ARG:HD3	1.87	0.42
2:B:25:LEU:HB3	2:B:30:PHE:HB2	2.01	0.42
2:B:589:LEU:HD21	2:B:608:LEU:HD23	2.01	0.42
1:A:203:PHE:CD1	1:A:203:PHE:N	2.87	0.42
2:B:215:LEU:HD11	2:B:272:ILE:HB	2.02	0.42
2:B:732:GLN:HB2	2:B:740:HIS:O	2.19	0.42
1:A:178:HIS:CB	1:A:218:GLN:HE22	2.33	0.41
1:A:180:SER:N	1:A:181:PRO:HD2	2.35	0.41
1:A:198:VAL:HA	1:A:199:PRO:HD2	1.87	0.41
1:A:184:VAL:HG13	1:A:294:VAL:HG22	2.02	0.41
1:A:87:ASP:O	1:A:90:LEU:HB2	2.20	0.41
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.35	0.41
2:B:609:LEU:HD13	2:B:652:LEU:CD1	2.50	0.41
1:A:178:HIS:HB2	6:A:1002:HOH:O	2.20	0.41
1:A:101:HIS:CE1	1:A:102:PRO:HD2	2.55	0.41
1:A:287:HIS:HB3	1:A:290:VAL:HG23	2.00	0.41
2:B:63:ARG:HD2	2:B:73:GLU:OE2	2.20	0.41
1:A:261:VAL:HG13	6:A:1001:HOH:O	2.21	0.41
2:B:706:PRO:HG2	2:B:709:GLU:HB2	2.02	0.41
2:B:468:GLY:HA3	2:B:470:GLU:OE2	2.21	0.41
2:B:624:PHE:CE1	2:B:642:VAL:HG13	2.56	0.41
1:A:198:VAL:HG22	1:A:198:VAL:O	2.20	0.41
1:A:245:PHE:HE2	1:A:269:VAL:HG21	1.86	0.41
1:A:103:ILE:CD1	1:A:320:GLU:HG3	2.49	0.41
2:B:309:PHE:HA	2:B:310:PRO:HD3	1.80	0.41
2:B:555:VAL:HG23	2:B:559:ASN:ND2	2.36	0.41
1:A:261:VAL:HG12	1:A:285:MET:C	2.42	0.41
2:B:446:PRO:HA	2:B:447:PRO:HD3	1.87	0.41
2:B:701:VAL:HG12	2:B:705:THR:HB	2.01	0.41
2:B:101:GLN:NE2	2:B:101:GLN:CA	2.79	0.41
2:B:166:ASP:O	2:B:172:GLY:HA3	2.21	0.41
2:B:72:VAL:HG21	2:B:89:LEU:HD11	2.03	0.41
2:B:96:LEU:HA	2:B:97:PRO:HD3	1.94	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:HIS:HB2	2:B:756:LEU:HD21	2.02	0.40
2:B:211:PRO:HD2	2:B:337:CYS:O	2.21	0.40
1:A:194:PHE:C	1:A:194:PHE:CD1	2.94	0.40
1:A:287:HIS:HA	1:A:288:PRO:HD3	1.97	0.40
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.56	0.40
2:B:577:PHE:N	2:B:577:PHE:CD1	2.89	0.40
2:B:601:GLU:CD	2:B:601:GLU:H	2.25	0.40
2:B:718:ALA:HB1	2:B:722:LEU:HD22	2.00	0.40
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.86	0.40
2:B:474:LEU:N	2:B:474:LEU:CD1	2.85	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:775:ARG:O	2:B:775:ARG:O[5_555]	1.86	0.34

## 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	264/266 (99%)	252 (96%)	11 (4%)	1 (0%)	34	57
2	B	783/785 (100%)	738 (94%)	40 (5%)	5 (1%)	25	47
All	All	1047/1051 (100%)	990 (95%)	51 (5%)	6 (1%)	25	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	100	GLY
2	B	244	ASN

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	102	LYS
2	B	97	PRO
2	B	761	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	214/214 (100%)	201 (94%)	13 (6%)	18	38
2	B	630/630 (100%)	584 (93%)	46 (7%)	14	28
All	All	844/844 (100%)	785 (93%)	59 (7%)	15	30

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	178	HIS
1	A	179	THR
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	205	PHE
1	A	213	GLU
1	A	260	PHE
1	A	261	VAL
1	A	308	ARG
1	A	321	ARG
2	B	32	THR
2	B	73	GLU
2	B	80	ASN
2	B	89	LEU
2	B	111	VAL
2	B	127	GLU
2	B	158	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	184	LEU
2	B	196	LEU
2	B	276	ARG
2	B	282	ARG
2	B	283	LEU
2	B	323	GLU
2	B	333	LEU
2	B	362	ARG
2	B	364	VAL
2	B	375	ARG
2	B	383	LEU
2	B	441	THR
2	B	445	THR
2	B	459	LEU
2	B	460	VAL
2	B	465	ARG
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	548	LEU
2	B	555	VAL
2	B	562	LEU
2	B	575	ARG
2	B	578	ARG
2	B	584	HIS
2	B	598	TRP
2	B	600	LYS
2	B	609	LEU
2	B	625	ARG
2	B	673	LEU
2	B	679	ASP
2	B	748	ARG
2	B	757	ARG
2	B	767	ARG
2	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	183	GLN
1	A	218	GLN
1	A	254	GLN
1	A	266	GLN
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	584	HIS
2	B	690	HIS
2	B	732	GLN
2	B	746	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	SO4	B	786	-	4,4,4	1.16	0	6,6,6	3.13	2 (33%)
4	YSA	A	999	-	35,38,38	2.36	10 (28%)	40,56,56	1.69	5 (12%)

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
4	YSA	A	999	-	-	4/18/39/39	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	YSA	OAD-SBI	6.54	1.48	1.42
4	A	999	YSA	C-NAT	5.98	1.48	1.37
4	A	999	YSA	O-C	-5.53	1.12	1.23
4	A	999	YSA	OAE-SBI	4.13	1.46	1.42
4	A	999	YSA	C8-N7	-3.17	1.29	1.34
4	A	999	YSA	C2-N3	2.91	1.36	1.32
4	A	999	YSA	CD1-CG	2.47	1.44	1.38
4	A	999	YSA	C2-N1	2.36	1.38	1.33
4	A	999	YSA	O4'-C1'	2.34	1.44	1.41
4	A	999	YSA	CD2-CG	2.27	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	YSA	C-NAT-SBI	-7.48	112.50	124.61
5	B	786	SO4	O4-S-O1	6.49	143.18	109.31
4	A	999	YSA	OAE-SBI-OAD	-4.17	114.26	120.76
5	B	786	SO4	O4-S-O3	-2.93	96.56	109.06
4	A	999	YSA	O5'-C5'-C4'	2.70	112.66	107.62
4	A	999	YSA	C3'-C2'-C1'	2.30	104.44	100.98
4	A	999	YSA	C4-C5-N7	2.25	111.75	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

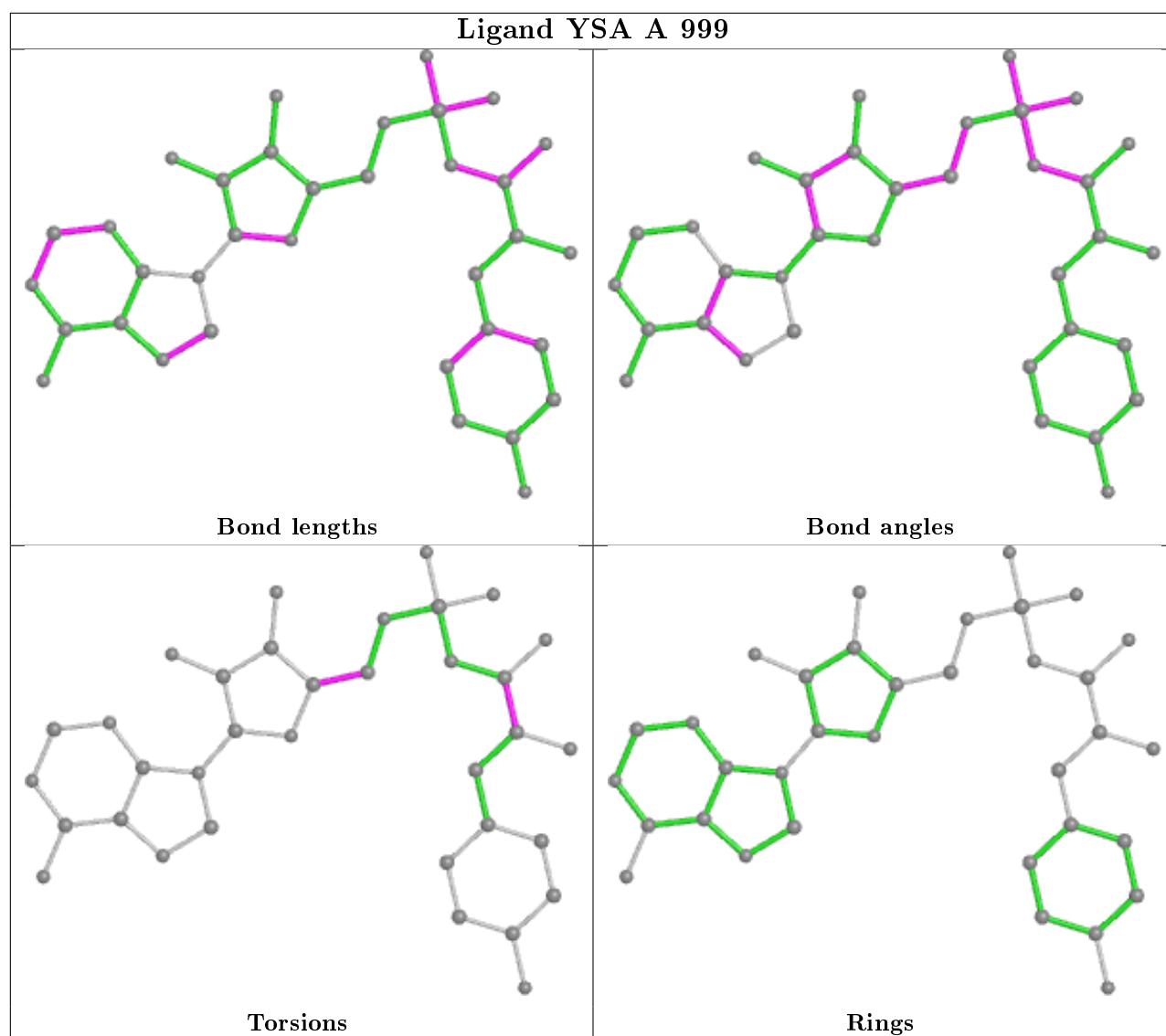
Mol	Chain	Res	Type	Atoms
4	A	999	YSA	O-C-CA-CB
4	A	999	YSA	NAT-C-CA-CB
4	A	999	YSA	O4'-C4'-C5'-O5'
4	A	999	YSA	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	YSA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/266 (100%)	-0.30	8 (3%)	50	43	20, 35, 68, 79	0
2	B	785/785 (100%)	-0.22	28 (3%)	42	35	18, 41, 81, 85	0
All	All	1051/1051 (100%)	-0.24	36 (3%)	45	38	18, 40, 79, 85	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	782	LEU	6.2
2	B	783	ASP	6.1
2	B	785	PRO	5.7
2	B	738	GLU	5.3
2	B	101	GLN	4.1
2	B	99	LEU	4.0
2	B	753	LYS	3.8
2	B	733	GLY	3.6
2	B	780	ARG	3.6
1	A	350	LEU	3.4
2	B	100	GLY	3.4
2	B	784	THR	3.3
2	B	98	GLY	3.1
2	B	781	GLY	3.0
2	B	736	LEU	3.0
2	B	731	TYR	2.9
2	B	689	ARG	2.9
2	B	43	ARG	2.9
1	A	273	GLU	2.9
2	B	306	GLU	2.8
2	B	767	ARG	2.8
2	B	759	GLU	2.7
2	B	734	PRO	2.5
2	B	735	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	757	ARG	2.5
1	A	278	LEU	2.4
2	B	739	GLY	2.3
1	A	142	HIS	2.2
1	A	168	GLU	2.2
2	B	732	GLN	2.2
2	B	601	GLU	2.1
2	B	34	ARG	2.1
1	A	275	GLY	2.1
2	B	60	ARG	2.0
1	A	207	GLN	2.0
1	A	85	ARG	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.

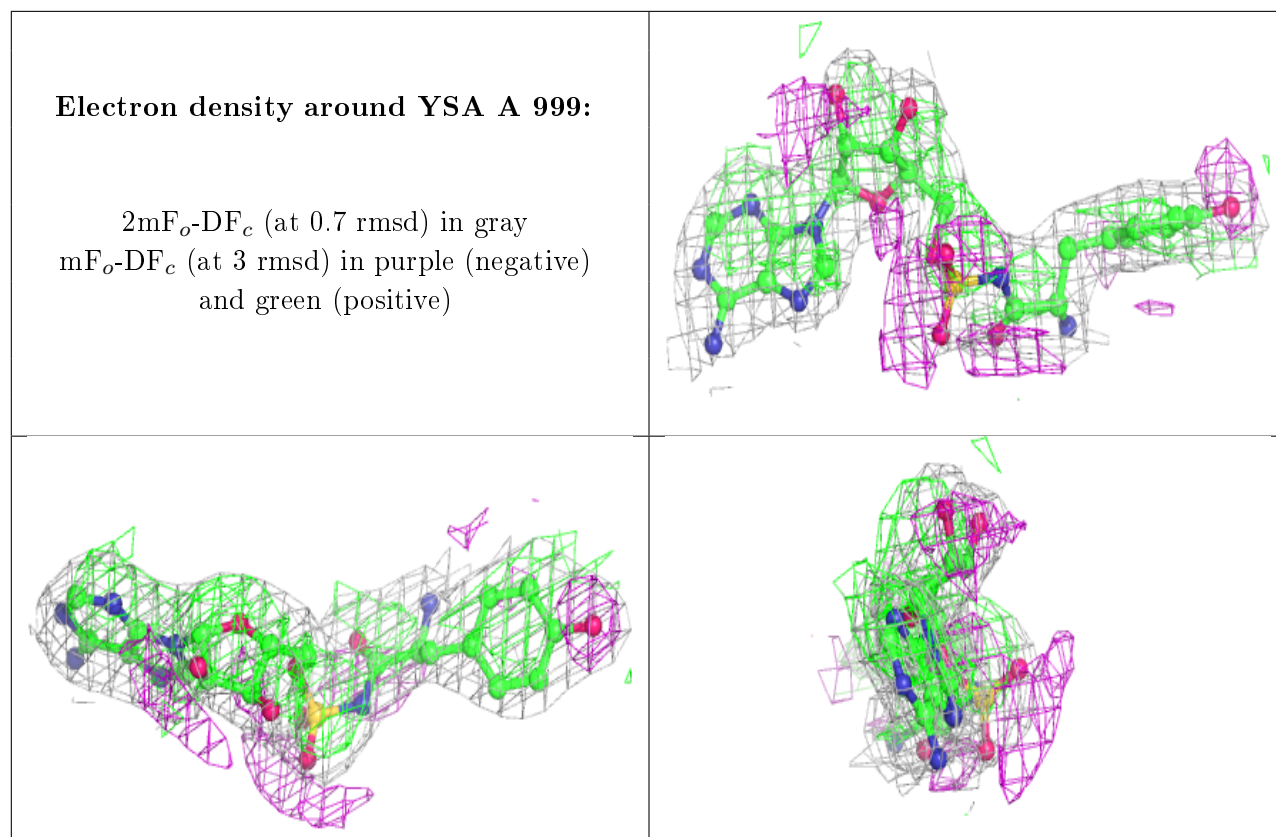
## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	A	901	1/1	0.85	0.34	43,43,43,43	0
4	YSA	A	999	35/35	0.86	0.29	6,60,68,69	0
5	SO4	B	786	5/5	0.88	0.49	5,5,5,5	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.