



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:01 AM UTC

PDB ID : 2ALY / pdb_00002aly
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

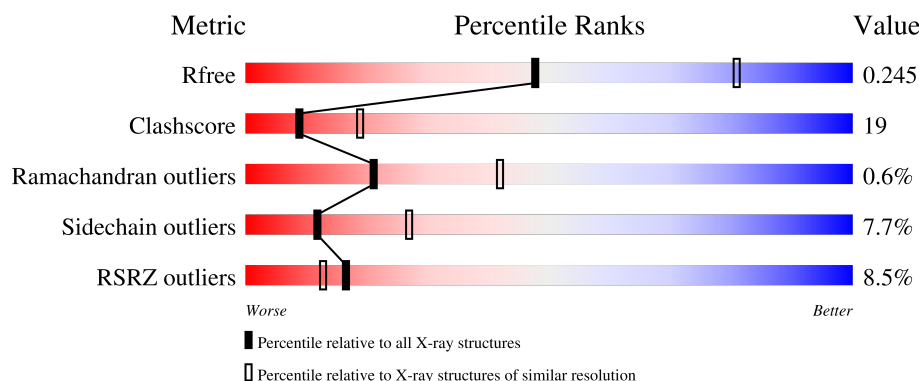
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	9% 65% 32% .
2	B	785	8% 62% 33% 5% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8522 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 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			

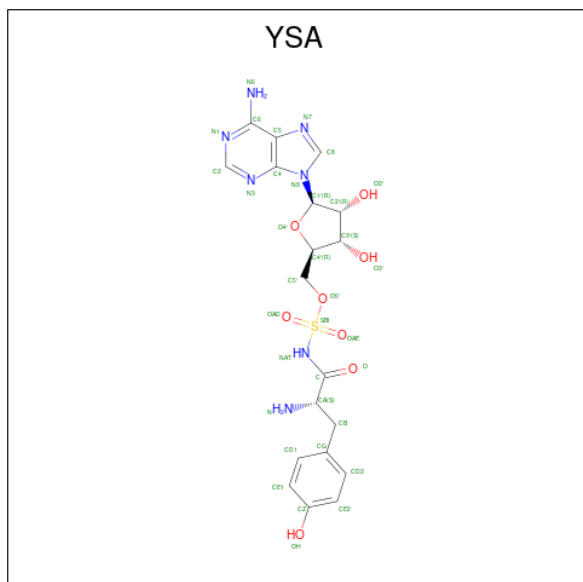
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

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 (CCD ID: MN) (formula: Mn).

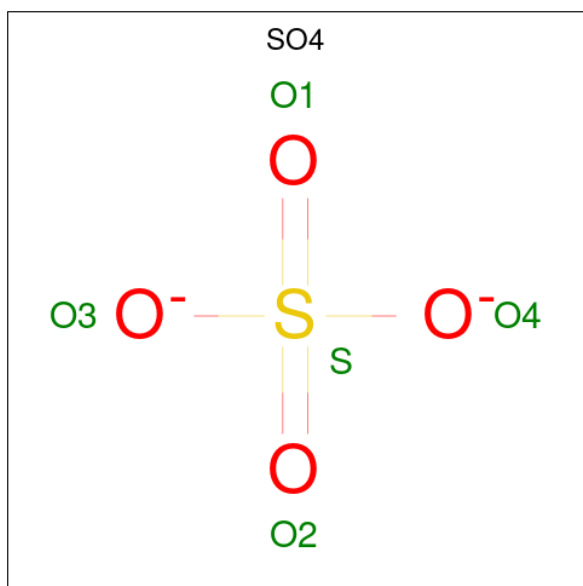
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5'-O-[N-(L-TYROSYL)SULFAMOYL]ADENOSINE (CCD ID: YSA) (formula: C₁₉H₂₃N₇O₈S).



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 (CCD ID: SO4) (formula: O₄S).



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

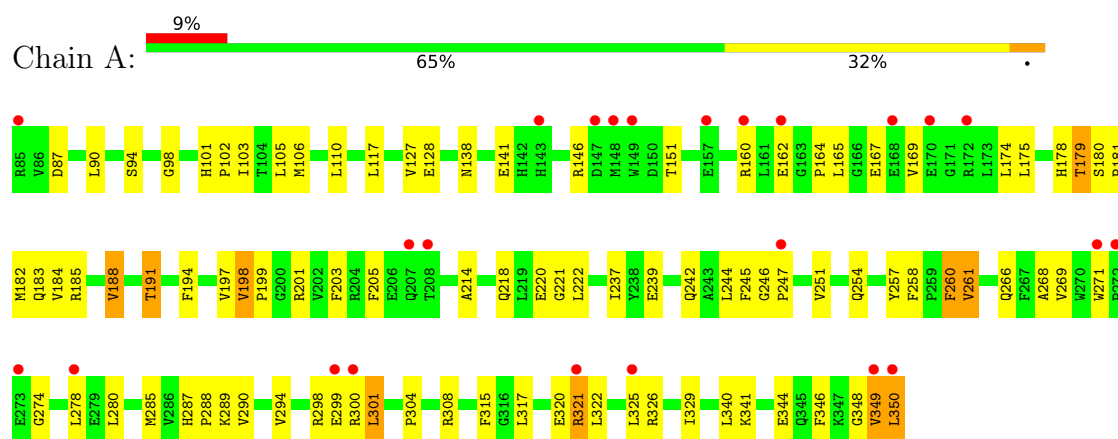
- Molecule 6 is water.

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

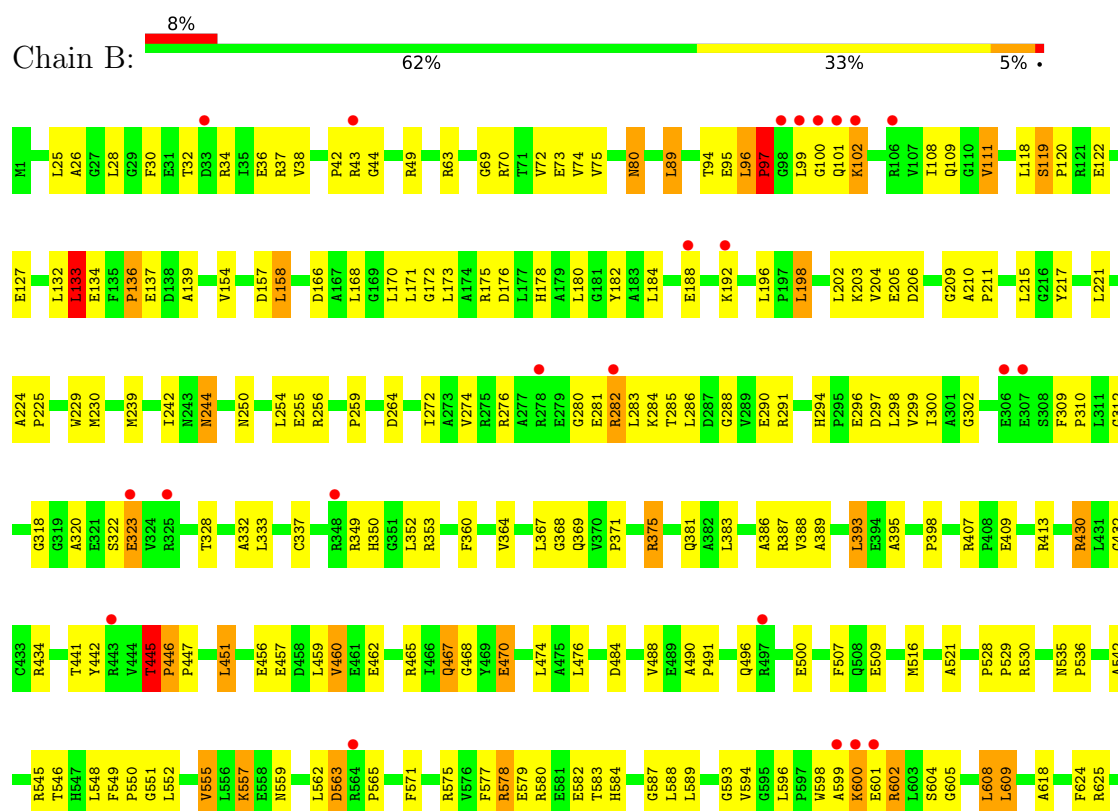
3 Residue-property plots

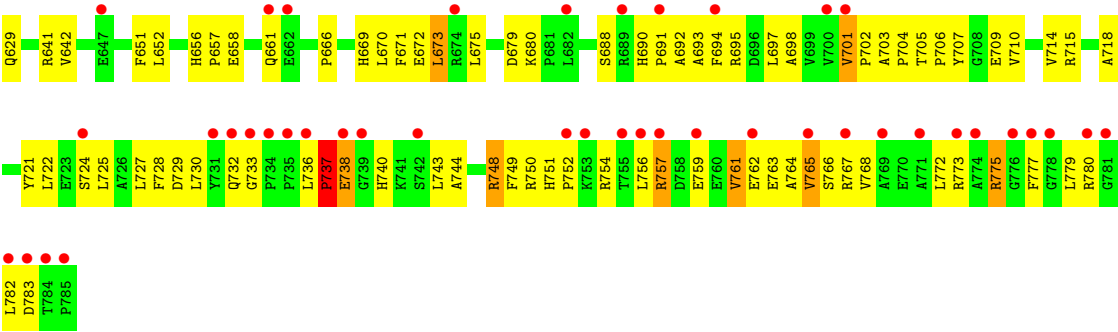
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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, α , β , γ	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) 99.8 (24.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.246 0.227 , 0.245	Depositor DCC
R_{free} test set	3757 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, YSA, 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	0.47	0/2191	0.97	10/2971 (0.3%)
2	B	0.44	0/6280	1.02	41/8536 (0.5%)
All	All	0.45	0/8471	1.01	51/11507 (0.4%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	15.50	128.72	113.53
2	B	118	LEU	N-CA-C	7.19	121.56	110.42
1	A	246	GLY	CA-C-N	6.93	127.51	119.47
1	A	246	GLY	C-N-CA	6.93	127.51	119.47
2	B	37	ARG	N-CA-C	-6.76	98.22	109.24
2	B	38	VAL	CB-CA-C	-6.75	104.03	110.65
2	B	738	GLU	CB-CA-C	6.68	118.99	109.71
1	A	214	ALA	N-CA-C	-6.46	105.21	113.23
2	B	387	ARG	N-CA-C	-6.46	98.72	109.24
2	B	242	ILE	N-CA-C	-6.27	106.66	111.62
2	B	445	THR	CA-C-N	6.18	126.75	120.38
2	B	445	THR	C-N-CA	6.18	126.75	120.38
1	A	329	ILE	CA-C-N	6.17	125.87	119.64
1	A	329	ILE	C-N-CA	6.17	125.87	119.64
1	A	151	THR	N-CA-C	6.01	119.69	110.20
2	B	521	ALA	N-CA-C	-5.99	104.88	111.82
2	B	528	PRO	CA-C-N	5.83	125.76	119.76
2	B	528	PRO	C-N-CA	5.83	125.76	119.76
2	B	96	LEU	CA-C-N	5.75	127.02	119.84
2	B	96	LEU	C-N-CA	5.75	127.02	119.84
2	B	563	ASP	N-CA-C	-5.72	100.71	109.41
2	B	119	SER	N-CA-C	-5.63	103.56	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	TYR	N-CA-C	5.60	118.60	109.59
2	B	666	PRO	N-CA-C	-5.59	103.88	110.70
2	B	393	LEU	N-CA-C	-5.58	100.20	109.46
2	B	446	PRO	CA-C-N	5.58	125.34	119.76
2	B	446	PRO	C-N-CA	5.58	125.34	119.76
2	B	737	PRO	CA-C-N	-5.56	112.89	121.56
2	B	737	PRO	C-N-CA	-5.56	112.89	121.56
2	B	136	PRO	N-CA-C	-5.55	102.47	111.19
1	A	266	GLN	N-CA-C	-5.53	100.88	109.72
2	B	618	ALA	N-CA-C	-5.51	104.91	111.69
2	B	70	ARG	N-CA-C	-5.46	101.97	110.42
2	B	701	VAL	N-CA-C	5.45	113.66	109.19
1	A	280	LEU	N-CA-C	5.44	118.04	111.40
2	B	168	LEU	N-CA-C	-5.42	106.70	113.15
2	B	442	TYR	N-CA-C	5.39	117.04	110.41
2	B	158	LEU	N-CA-C	5.35	118.54	109.76
2	B	670	LEU	N-CA-C	5.33	115.58	108.38
2	B	680	LYS	CA-C-N	5.28	125.53	119.83
2	B	680	LYS	C-N-CA	5.28	125.53	119.83
2	B	69	GLY	N-CA-C	-5.22	100.80	113.18
2	B	302	GLY	N-CA-C	-5.20	103.17	111.18
2	B	322	SER	N-CA-C	5.19	120.53	113.37
2	B	210	ALA	CA-C-N	5.16	125.46	119.47
2	B	210	ALA	C-N-CA	5.16	125.46	119.47
2	B	332	ALA	N-CA-C	-5.16	100.11	108.52
2	B	133	LEU	N-CA-C	-5.12	102.71	110.28
2	B	388	VAL	N-CA-C	5.09	115.81	108.48
1	A	260	PHE	N-CA-C	5.05	119.42	113.16
2	B	608	LEU	N-CA-C	-5.00	105.30	111.40

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	2123	0	2075	75	0
2	B	6127	0	6180	243	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
All	All	8522	0	8277	308	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 19.

All (308) 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:239:MET:HE2	2:B:254:LEU:HD11	1.63	0.80
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:80:ASN:H	2:B:80:ASN:HD22	1.29	0.78
2:B:600:LYS:HD3	2:B:600:LYS:H	1.48	0.78
2:B:101:GLN:HE21	2:B:101:GLN:HA	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: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:HG2	2:B:575:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD21	1:A:322:LEU:HD21	1.71	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
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:HE	2:B:767:ARG:N	1.94	0.65
2:B:602:ARG:HG3	2:B:602:ARG:NH1	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:702:PRO:C	2:B:704:PRO:HD2	2.23	0.64
2:B:737:PRO:O	2:B:738:GLU:C	2.38	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:HA	2:B:467:GLN:NE2	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:588:LEU:C	2:B:588:LEU:HD23	2.24	0.62
2:B:761:VAL:O	2:B:765:VAL:HG13	1.99	0.62
2:B:284:LYS:HZ1	2:B:288:GLY:HA2	1.65	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:HD22	2:B:80:ASN:N	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:432:GLY:C	2:B:447:PRO:HG3	2.27	0.60
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:O	2:B:101:GLN:N	2.37	0.58
2:B:353:ARG:C	2:B:353:ARG:HD3	2.29	0.58
2:B:730:LEU:HD13	2:B:743:LEU:CD2	2.33	0.58
2:B:286:LEU:HD21	2:B:323:GLU:HG2	1.83	0.58
2:B:224:ALA:N	2:B:244:ASN:HD22	2.02	0.57
1:A:317:LEU:C	1:A:317:LEU:HD12	2.30	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
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.69	0.57
2:B:575:ARG:HG2	2:B:575:ARG:NH1	2.19	0.57
2:B:672:GLU:C	2:B:673:LEU:HD23	2.30	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:101:GLN:O	2:B:102:LYS:C	2.48	0.56
2:B:701:VAL:CG1	2:B:705:THR:HB	2.34	0.56
1:A:174:LEU:C	1:A:174:LEU:HD12	2.30	0.56
1:A:180:SER:O	1:A:183:GLN:HB3	2.05	0.56
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.19	0.56
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.88	0.56
2:B:516:MET:HE3	2:B:545:ARG:HA	1.88	0.56
1:A:138:ASN:OD1	1:A:289:LYS:HE3	2.06	0.56
2:B:239:MET:HE2	2:B:254:LEU:CD1	2.35	0.55
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:297:ASP:OD2	2:B:350:HIS:HE1	1.90	0.55
2:B:516:MET:HE3	2:B:546:THR:H	1.72	0.55
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.88	0.55
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.14	0.55
2:B:462:GLU:CD	2:B:465:ARG:NH1	2.65	0.55
2:B:604:SER:HA	2:B:608:LEU:HD22	1.87	0.55
2:B:43:ARG:HG3	2:B:43:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:VAL:HG13	2:B:777:PHE:CE1	2.43	0.53
2:B:703:ALA:N	2:B:704:PRO:HD2	2.23	0.53
2:B:629:GLN:OE1	2:B:641:ARG:HD3	2.07	0.53
2:B:697:LEU:C	2:B:697:LEU:HD12	2.33	0.53
2:B:732:GLN:O	2:B:732:GLN:HG3	2.07	0.53
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.43	0.53
2:B:368:GLY:C	2:B:371:PRO:HD2	2.33	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:HD23	2:B:198:LEU:N	2.23	0.53
2:B:367:LEU:HD21	2:B:398:PRO:HB2	1.91	0.53
2:B:563:ASP:C	2:B:565:PRO:HD3	2.34	0.53
1:A:258:PHE:CE2	4:A:999:YSA:HD1	2.43	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
2:B:229:TRP:CH2	2:B:230:MET:HE3	2.45	0.52
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:368:GLY:O	2:B:371:PRO:HD2	2.10	0.52
2:B:698:ALA:O	2:B:779:LEU:HD12	2.10	0.52
2:B:759:GLU:O	2:B:763:GLU:HB2	2.10	0.52
2:B:299:VAL:HG11	2:B:310:PRO:HB3	1.91	0.52
2:B:34:ARG:HG2	2:B:34:ARG:HH11	1.75	0.52
2:B:692:ALA:HB2	2:B:750:ARG:HD2	1.92	0.52
2:B:697:LEU:HD12	2:B:697:LEU:O	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
2:B:693:ALA:O	2:B:748:ARG:HA	2.10	0.51
2:B:99:LEU:C	2:B:101:GLN:H	2.18	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
1:A:205:PHE:HD2	2:B:535:ASN:HD22	1.59	0.50
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.41	0.50
2:B:434:ARG:HB3	2:B:445:THR:HG23	1.93	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:549:PHE:O	2:B:550:PRO:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:202:LEU:HB2	2:B:393:LEU:HD23	1.95	0.49
2:B:221:LEU:HD23	2:B:386:ALA:HB2	1.94	0.49
1:A:348:GLY:O	1:A:350:LEU:N	2.46	0.49
2:B:552:LEU:O	2:B:555:VAL:HG13	2.13	0.48
2:B:369:GLN:CD	2:B:369:GLN:H	2.21	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:HD12	1:A:317:LEU:O	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:281:GLU:HG2	2:B:310:PRO:HG2	1.96	0.47
1:A:326:ARG:NH1	1:A:326:ARG:HG3	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
1:A:106:MET:HE3	1:A:106:MET:HA	1.97	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:509:GLU:HB2	2:B:571:PHE:CE1	2.50	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:36:GLU:O	2:B:154:VAL:HA	2.15	0.47
2:B:96:LEU:HB2	2:B:99:LEU:HG	1.96	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:609:LEU:HD13	2:B:652:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:600:LYS:HG2	2:B:601:GLU:CD	2.40	0.46
2:B:602:ARG:NH1	2:B:602:ARG:CG	2.75	0.46
2:B:80:ASN:H	2:B:80:ASN:ND2	2.07	0.45
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.46	0.45
1:A:261:VAL:HG12	1:A:285:MET:C	2.42	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:49:ARG:HG3	2:B:137:GLU:HG3	1.98	0.45
2:B:299:VAL:HG12	2:B:300:ILE:N	2.31	0.45
1:A:254:GLN:NE2	2:B:26:ALA:HB1	2.31	0.45
2:B:451:LEU:HD23	2:B:451:LEU:N	2.32	0.45
2:B:601:GLU:CD	2:B:601:GLU:H	2.25	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
1:A:194:PHE:CD1	1:A:194:PHE:C	2.94	0.45
2:B:175:ARG:O	2:B:178:HIS:HB3	2.17	0.45
2:B:323:GLU:OE2	2:B:323:GLU:CA	2.64	0.45
2:B:457:GLU:O	2:B:460:VAL:HG13	2.17	0.44
1:A:98:GLY:HA3	2:B:507:PHE:O	2.17	0.44
6:A:1014:HOH:O	2:B:476:LEU:HD23	2.17	0.44
2:B:718:ALA:O	2:B:749:PHE:HE2	2.01	0.44
1:A:191:THR:CG2	2:B:484:ASP:OD2	2.56	0.44
2:B:136:PRO:HD2	2:B:139:ALA:HB2	1.99	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:HG3	2:B:43:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:409:GLU:CD	2:B:413:ARG:HH11	2.26	0.43
1:A:94:SER:O	2:B:594:VAL:HG13	2.17	0.43
1:A:164:PRO:HD2	1:A:167:GLU:OE2	2.19	0.43
2:B:715:ARG:HB2	2:B:715:ARG:NH1	2.33	0.43
2:B:578:ARG:C	2:B:580:ARG:H	2.26	0.43
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.54	0.43
1:A:349:VAL:C	1:A:350:LEU:HD22	2.44	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:516:MET:CE	2:B:546:THR:H	2.31	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
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
2:B:239:MET:HE1	2:B:250:ASN:HB3	2.01	0.42
1:A:164:PRO:HG2	1:A:188:VAL:HG21	2.02	0.42
1:A:299:GLU:O	1:A:300:ARG:C	2.63	0.42
2:B:192:LYS:O	2:B:192:LYS:HD3	2.18	0.42
2:B:729:ASP:HB3	2:B:744:ALA:HB3	2.02	0.42
2:B:108:ILE:O	2:B:109:GLN:C	2.63	0.42
2:B:757:ARG:HD3	2:B:757:ARG:HA	1.87	0.42
2:B:25:LEU:HB3	2:B:30:PHE:HB2	2.01	0.42
2:B:651:PHE:C	2:B:651:PHE:CD1	2.97	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
2:B:516:MET:HE1	2:B:546:THR:OG1	2.19	0.41
2:B:782:LEU:HD23	2:B:782:LEU:C	2.45	0.41
1:A:87:ASP:O	1:A:90:LEU:HB2	2.20	0.41
1:A:184:VAL:HG13	1:A:294:VAL:HG22	2.02	0.41
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:PHE:CD1	1:A:205:PHE:C	2.98	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
2:B:264:ASP:CG	2:B:328:THR:HG23	2.46	0.41
2:B:462:GLU:CD	2:B:465:ARG:HH12	2.21	0.41
1:A:261:VAL:HG13	6:A:1001:HOH:O	2.21	0.41
2:B:557:LYS:C	2:B:557:LYS:HD3	2.46	0.41
2:B:706:PRO:HG2	2:B:709:GLU:HB2	2.02	0.41
2:B:280:GLY:O	2:B:281:GLU:C	2.63	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:103:ILE:CD1	1:A:320:GLU:HG3	2.49	0.41
1:A:198:VAL:O	1:A:198:VAL:HG22	2.20	0.41
1:A:245:PHE:HE2	1:A:269:VAL:HG21	1.86	0.41
2:B:309:PHE:HA	2:B:310:PRO:HD3	1.80	0.41
2:B:446:PRO:HA	2:B:447:PRO:HD3	1.87	0.41
2:B:555:VAL:HG23	2:B:559:ASN:ND2	2.36	0.41
2:B:701:VAL:HG12	2:B:705:THR:HB	2.01	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
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:764:ALA:C	2:B:766:SER:N	2.78	0.41
2:B:209:GLY:C	2:B:211:PRO:HD3	2.46	0.40
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: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:CD1	2:B:577:PHE:N	2.89	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%)	30	51
2	B	783/785 (100%)	738 (94%)	40 (5%)	5 (1%)	21	42
All	All	1047/1051 (100%)	990 (95%)	51 (5%)	6 (1%)	21	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	100	GLY
2	B	244	ASN
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%)	199 (93%)	15 (7%)	14	31
2	B	630/630 (100%)	580 (92%)	50 (8%)	11	26
All	All	844/844 (100%)	779 (92%)	65 (8%)	12	27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	169	VAL
1	A	179	THR
1	A	188	VAL
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	260	PHE
1	A	261	VAL
1	A	301	LEU
1	A	308	ARG
1	A	321	ARG
1	A	341	LYS
1	A	350	LEU
2	B	32	THR
2	B	74	VAL
2	B	80	ASN
2	B	89	LEU
2	B	97	PRO
2	B	111	VAL
2	B	127	GLU
2	B	133	LEU
2	B	158	LEU
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	198	LEU
2	B	282	ARG
2	B	283	LEU
2	B	323	GLU
2	B	333	LEU
2	B	364	VAL
2	B	375	ARG
2	B	383	LEU
2	B	430	ARG
2	B	441	THR
2	B	445	THR
2	B	451	LEU
2	B	459	LEU

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Mol	Chain	Res	Type
2	B	460	VAL
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	548	LEU
2	B	555	VAL
2	B	557	LYS
2	B	562	LEU
2	B	578	ARG
2	B	598	TRP
2	B	600	LYS
2	B	602	ARG
2	B	609	LEU
2	B	625	ARG
2	B	673	LEU
2	B	679	ASP
2	B	725	LEU
2	B	737	PRO
2	B	748	ARG
2	B	757	ARG
2	B	765	VAL
2	B	775	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	183	GLN
1	A	190	HIS
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

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Mol	Chain	Res	Type
2	B	485	ASN
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 oligosaccharides 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	$\# Z > 2$
4	YSA	A	999	-	38,38,38	2.28	10 (26%)	53,56,56	1.29	6 (11%)
5	SO4	B	786	-	4,4,4	1.06	0	6,6,6	3.01	2 (33%)

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	-	-	4/22/39/39	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	6.35	1.48	1.42
4	A	999	YSA	C-NAT	6.24	1.48	1.37
4	A	999	YSA	O-C	-5.73	1.12	1.23
4	A	999	YSA	OAE-SBI	4.02	1.46	1.42
4	A	999	YSA	CD1-CG	2.66	1.44	1.38
4	A	999	YSA	C2-N1	2.46	1.38	1.33
4	A	999	YSA	CD2-CG	2.44	1.43	1.38
4	A	999	YSA	C5-C6	2.42	1.47	1.41
4	A	999	YSA	CE1-CD1	2.16	1.42	1.38
4	A	999	YSA	C1'-N9	2.14	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	786	SO4	O4-S-O1	6.43	143.18	109.56
4	A	999	YSA	OAE-SBI-OAD	-4.40	114.26	120.85
4	A	999	YSA	C-NAT-SBI	-3.16	112.50	124.07
4	A	999	YSA	O5'-C5'-C4'	2.86	112.66	107.57
4	A	999	YSA	O4'-C1'-N9	-2.44	103.41	108.09
4	A	999	YSA	C6-C5-C4	-2.28	114.07	117.18
5	B	786	SO4	O4-S-O3	-2.17	96.56	108.54
4	A	999	YSA	N9-C8-N7	2.09	116.91	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

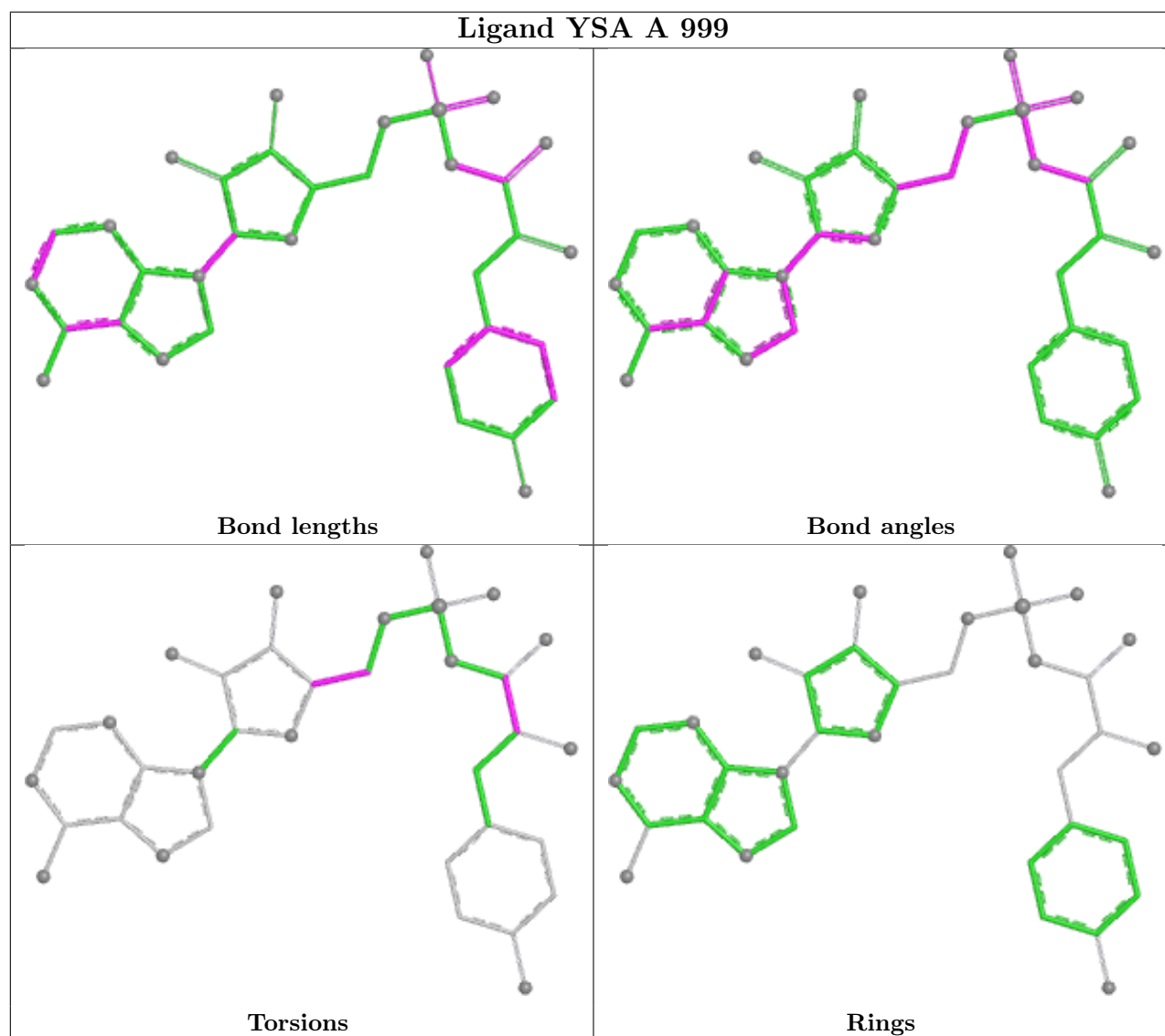
Mol	Chain	Res	Type	Atoms
4	A	999	YSA	O-C-CA-CB
4	A	999	YSA	NAT-C-CA-CB
4	A	999	YSA	O4'-C4'-C5'-O5'
4	A	999	YSA	C3'-C4'-C5'-O5'

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	266/266 (100%)	0.07	24 (9%)	15 11	20, 35, 68, 79	0
2	B	785/785 (100%)	0.26	65 (8%)	17 13	18, 41, 81, 85	0
All	All	1051/1051 (100%)	0.21	89 (8%)	16 13	18, 40, 79, 85	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	8.6
2	B	782	LEU	8.2
2	B	785	PRO	6.4
2	B	783	ASP	5.8
2	B	99	LEU	5.8
2	B	738	GLU	5.7
2	B	724	SER	5.6
2	B	784	THR	5.3
2	B	781	GLY	5.1
2	B	689	ARG	4.9
2	B	100	GLY	4.6
1	A	278	LEU	4.5
2	B	101	GLN	4.4
2	B	564	ARG	4.2
2	B	780	ARG	3.9
1	A	273	GLU	3.8
2	B	731	TYR	3.8
2	B	736	LEU	3.5
2	B	767	ARG	3.5
2	B	325	ARG	3.5
1	A	349	VAL	3.4
2	B	661	GLN	3.3
2	B	307	GLU	3.3
2	B	734	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	102	LYS	3.2
1	A	85	ARG	3.2
2	B	753	LYS	3.2
2	B	733	GLY	3.1
1	A	160	ARG	3.0
2	B	98	GLY	3.0
2	B	600	LYS	3.0
2	B	757	ARG	3.0
2	B	778	GLY	3.0
2	B	755	THR	2.8
2	B	106	ARG	2.8
1	A	149	TRP	2.8
1	A	271	TRP	2.7
2	B	601	GLU	2.7
2	B	771	ALA	2.7
2	B	497	ARG	2.7
2	B	759	GLU	2.7
2	B	735	PRO	2.7
2	B	732	GLN	2.7
2	B	739	GLY	2.7
1	A	325	LEU	2.6
1	A	157	GLU	2.6
1	A	272	PRO	2.6
2	B	682	LEU	2.5
2	B	443	ARG	2.5
2	B	776	GLY	2.5
2	B	701	VAL	2.5
1	A	168	GLU	2.5
2	B	769	ALA	2.5
2	B	694	PHE	2.4
2	B	43	ARG	2.4
2	B	323	GLU	2.4
2	B	192	LYS	2.4
2	B	762	GLU	2.4
1	A	162	GLU	2.3
1	A	170	GLU	2.3
1	A	147	ASP	2.3
2	B	742	SER	2.3
2	B	756	LEU	2.3
2	B	188	GLU	2.3
2	B	647	GLU	2.3
1	A	247	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	752	PRO	2.3
1	A	207	GLN	2.3
2	B	599	ALA	2.3
1	A	172	ARG	2.3
2	B	700	VAL	2.3
2	B	765	VAL	2.3
1	A	143	HIS	2.3
2	B	773	ARG	2.2
2	B	691	PRO	2.2
2	B	33	ASP	2.2
1	A	299	GLU	2.2
1	A	208	THR	2.2
2	B	282	ARG	2.2
2	B	306	GLU	2.1
2	B	662	GLU	2.1
1	A	148	MET	2.1
1	A	300	ARG	2.1
1	A	321	ARG	2.1
2	B	278	ARG	2.1
2	B	777	PHE	2.1
2	B	774	ALA	2.0
2	B	348	ARG	2.0
2	B	674	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

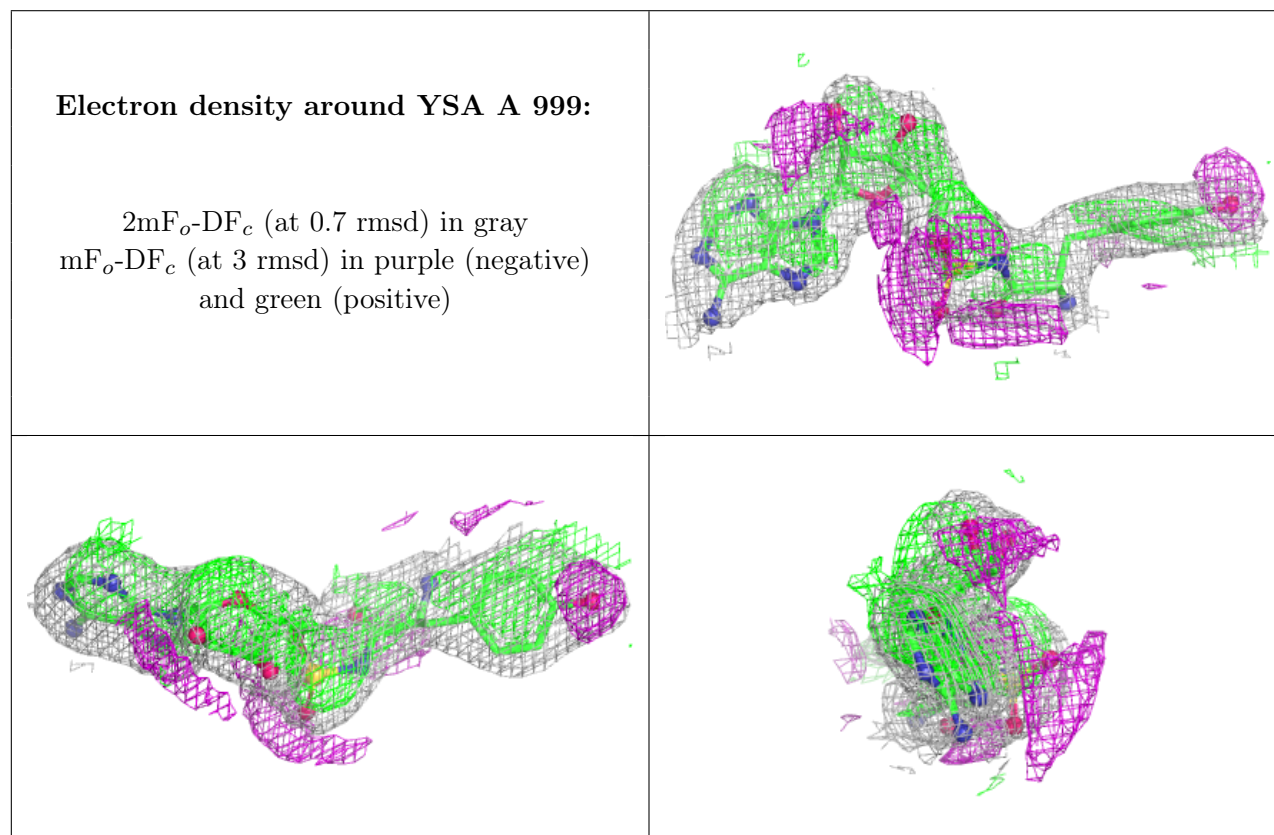
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	A	901	1/1	0.64	0.28	43,43,43,43	0
4	YSA	A	999	35/35	0.83	0.27	6,60,68,69	0
5	SO4	B	786	5/5	0.87	0.45	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 ⓘ

There are no such residues in this entry.