



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:13 PM UTC

PDB ID : 3KT8 / pdb_00003kt8
Title : Crystal structure of *S. cerevisiae* tryptophanyl-tRNA synthetase in complex with L-tryptophanamide
Authors : Zhou, M.; Dong, X.; Zhong, C.; Shen, N.; Ding, J.
Deposited on : 2009-11-24
Resolution : 3.00 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
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

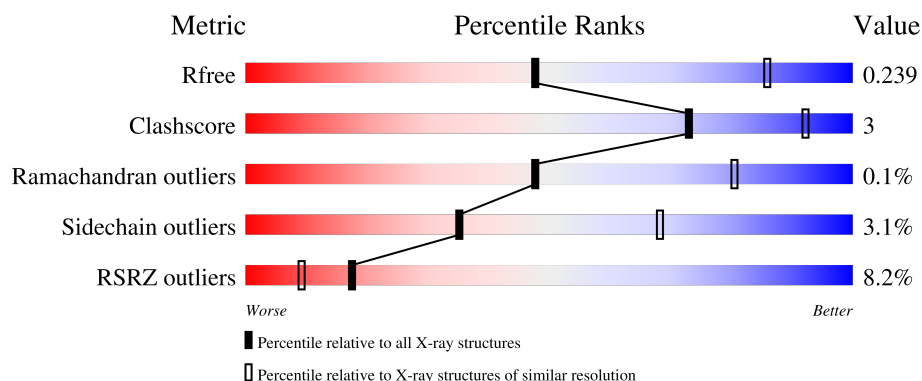
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	438	6% 81% 12% 7%
1	B	438	8% 83% 9% 8%
1	C	438	8% 83% 9% 8%
1	D	438	8% 82% 10% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13222 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 Tryptophanyl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3287	2118	545	611	13			
1	B	403	Total	C	N	O	S	0	0	0
			3250	2096	539	602	13			
1	C	403	Total	C	N	O	S	0	0	0
			3250	2096	539	602	13			
1	D	410	Total	C	N	O	S	0	0	0
			3304	2129	547	615	13			

There are 24 discrepancies between the modelled and reference sequences:

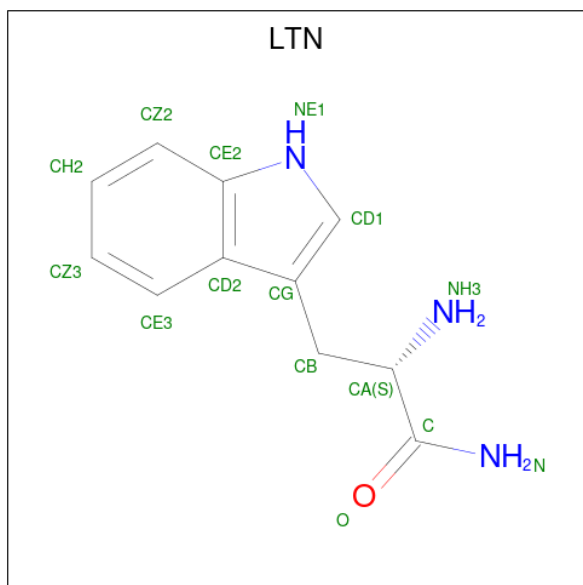
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	HIS	-	expression tag	UNP Q12109
A	434	HIS	-	expression tag	UNP Q12109
A	435	HIS	-	expression tag	UNP Q12109
A	436	HIS	-	expression tag	UNP Q12109
A	437	HIS	-	expression tag	UNP Q12109
A	438	HIS	-	expression tag	UNP Q12109
B	433	HIS	-	expression tag	UNP Q12109
B	434	HIS	-	expression tag	UNP Q12109
B	435	HIS	-	expression tag	UNP Q12109
B	436	HIS	-	expression tag	UNP Q12109
B	437	HIS	-	expression tag	UNP Q12109
B	438	HIS	-	expression tag	UNP Q12109
C	433	HIS	-	expression tag	UNP Q12109
C	434	HIS	-	expression tag	UNP Q12109
C	435	HIS	-	expression tag	UNP Q12109
C	436	HIS	-	expression tag	UNP Q12109
C	437	HIS	-	expression tag	UNP Q12109
C	438	HIS	-	expression tag	UNP Q12109
D	433	HIS	-	expression tag	UNP Q12109
D	434	HIS	-	expression tag	UNP Q12109
D	435	HIS	-	expression tag	UNP Q12109

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Chain	Residue	Modelled	Actual	Comment	Reference
D	436	HIS	-	expression tag	UNP Q12109
D	437	HIS	-	expression tag	UNP Q12109
D	438	HIS	-	expression tag	UNP Q12109

- Molecule 2 is L-TRYPTOPHANAMIDE (CCD ID: LTN) (formula: $C_{11}H_{13}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	3	1		
2	B	1	Total	C	N	O	0	0
			15	11	3	1		
2	C	1	Total	C	N	O	0	0
			15	11	3	1		
2	D	1	Total	C	N	O	0	0
			15	11	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

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

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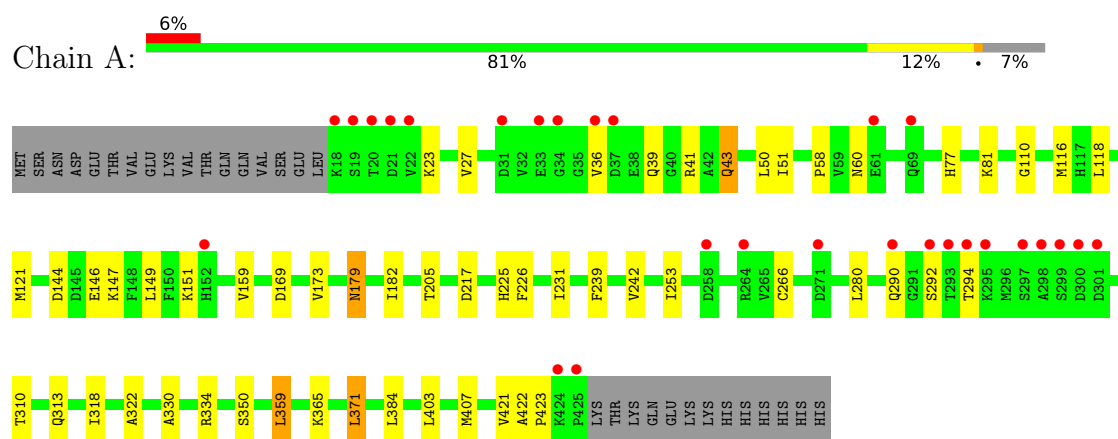
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	D	8	Total	O	0	0
			8	8		

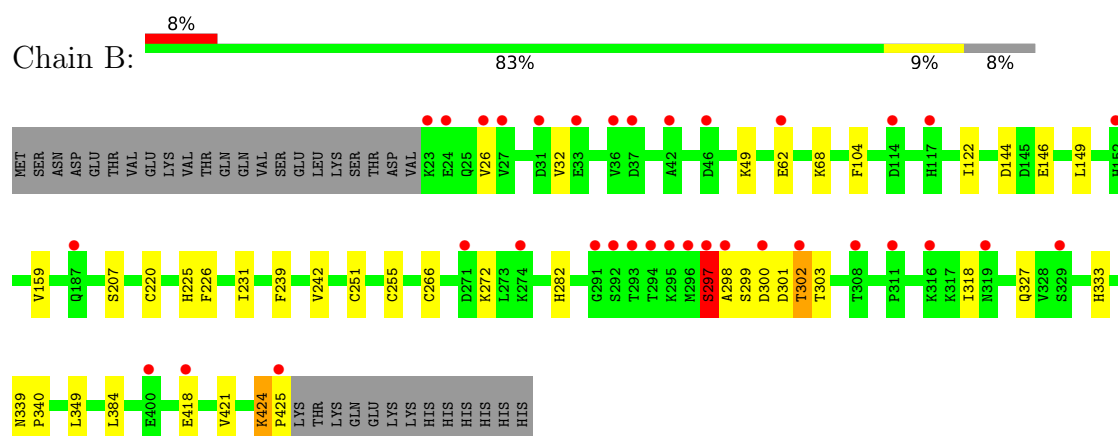
3 Residue-property plots [i](#)

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.

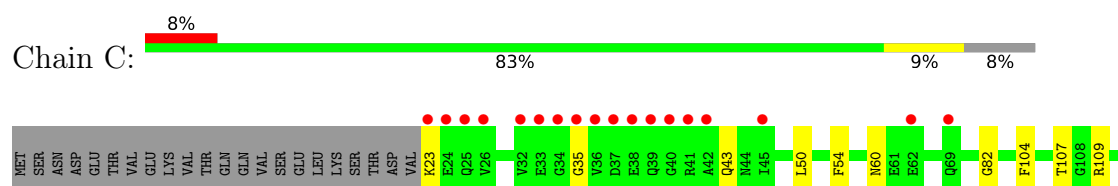
- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

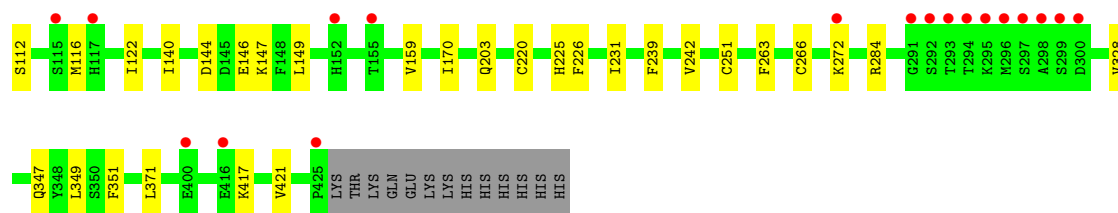


- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

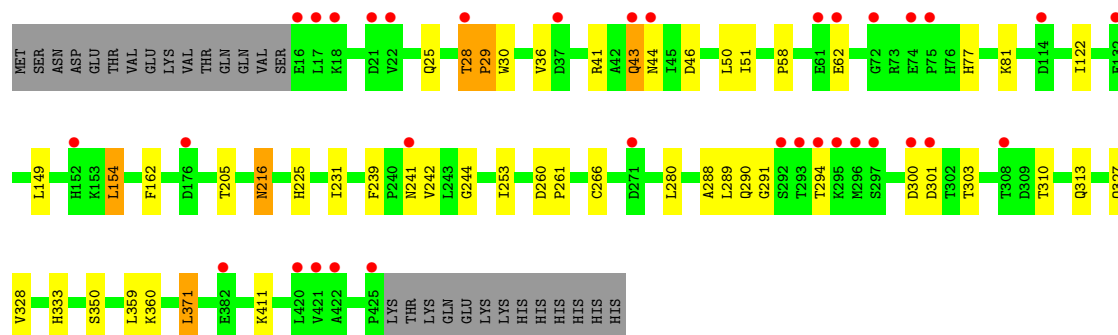
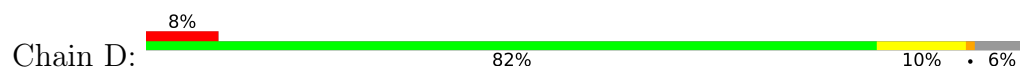


- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic





● Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	252.26Å 252.26Å 111.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.04 – 3.00 49.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.04-3.00) 97.7 (49.04-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.273 0.240 , 0.239	Depositor DCC
R_{free} test set	3960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13222	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/3369	0.77	0/4546
1	B	0.42	1/3332 (0.0%)	0.82	2/4496 (0.0%)
1	C	0.42	1/3332 (0.0%)	0.76	0/4496
1	D	0.42	1/3386 (0.0%)	0.79	0/4569
All	All	0.42	3/13419 (0.0%)	0.78	2/18107 (0.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	ILE	CA-CB	5.97	1.57	1.54
1	C	122	ILE	CA-CB	5.68	1.56	1.54
1	B	122	ILE	CA-CB	5.36	1.57	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	ALA	N-CA-C	-19.20	87.45	112.41
1	B	297	SER	N-CA-C	-6.24	100.17	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	SER	Peptide

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	3287	0	3247	29	0
1	B	3250	0	3209	19	0
1	C	3250	0	3209	17	0
1	D	3304	0	3264	24	0
2	A	15	0	13	0	0
2	B	15	0	13	0	0
2	C	15	0	13	0	0
2	D	15	0	13	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	1	0	0	0	0
4	D	8	0	0	0	0
All	All	13222	0	12981	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:THR:H	1:A:313:GLN:HE21	1.28	0.79
1:D:28:THR:HG22	1:D:29:PRO:HD2	1.71	0.72
1:C:109:ARG:HG2	1:C:116:MET:HE2	1.79	0.64
1:A:179:ASN:H	1:A:179:ASN:HD22	1.45	0.64
1:C:239:PHE:HB3	1:C:242:VAL:HB	1.81	0.63
1:D:288:ALA:HB3	1:D:294:THR:HG23	1.82	0.62
1:D:333:HIS:HE1	1:D:371:LEU:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HB3	1:A:36:VAL:H	1.68	0.59
1:A:110:GLY:HA3	1:A:147:LYS:HE3	1.84	0.59
1:B:239:PHE:HB3	1:B:242:VAL:HB	1.83	0.58
1:D:350:SER:HA	1:D:359:LEU:HD21	1.86	0.58
1:B:299:SER:HB2	1:B:303:THR:OG1	2.04	0.57
1:B:297:SER:C	1:B:299:SER:H	2.00	0.57
1:A:121:MET:HE1	1:A:173:VAL:HG22	1.87	0.54
1:A:330:ALA:O	1:A:334:ARG:HG2	2.07	0.54
1:B:327:GLN:H	1:B:333:HIS:HD2	1.54	0.54
1:C:220:CYS:HA	1:D:205:THR:HA	1.90	0.52
1:A:77:HIS:HB2	1:A:81:LYS:HE3	1.91	0.52
1:D:260:ASP:N	1:D:261:PRO:HD2	2.24	0.52
1:C:50:LEU:O	1:C:54:PHE:HB2	2.10	0.52
1:D:77:HIS:HB2	1:D:81:LYS:HE3	1.90	0.52
1:A:239:PHE:HB3	1:A:242:VAL:HB	1.91	0.52
1:C:112:SER:HB3	1:C:147:LYS:HD2	1.92	0.51
1:B:231:ILE:HG12	1:B:266:CYS:HB2	1.93	0.51
1:B:327:GLN:H	1:B:333:HIS:CD2	2.28	0.51
1:A:350:SER:HA	1:A:359:LEU:HD21	1.92	0.50
1:C:116:MET:HE1	1:C:170:ILE:HG13	1.94	0.50
1:C:144:ASP:HB2	1:C:159:VAL:HB	1.94	0.50
1:D:327:GLN:H	1:D:333:HIS:CD2	2.30	0.50
1:D:36:VAL:HA	1:D:41:ARG:HA	1.95	0.49
1:A:182:ILE:O	1:A:407:MET:HA	2.13	0.48
1:D:253:ILE:HB	1:D:280:LEU:HD23	1.94	0.48
1:A:116:MET:HE2	1:A:169:ASP:HB3	1.96	0.48
1:B:318:ILE:HD11	1:B:384:LEU:HD12	1.94	0.48
1:A:225:HIS:HB2	1:B:225:HIS:HB2	1.96	0.48
1:D:327:GLN:H	1:D:333:HIS:HD2	1.62	0.48
1:A:144:ASP:HB2	1:A:159:VAL:HB	1.95	0.47
1:B:418:GLU:H	1:B:418:GLU:CD	2.22	0.47
1:A:51:ILE:HD13	1:A:58:PRO:HB3	1.95	0.47
1:A:310:THR:H	1:A:313:GLN:NE2	2.06	0.47
1:B:300:ASP:O	1:B:302:THR:N	2.41	0.47
1:D:310:THR:H	1:D:313:GLN:HE21	1.63	0.46
1:A:365:LYS:HB3	1:A:371:LEU:HB2	1.98	0.46
1:A:36:VAL:HA	1:A:41:ARG:HA	1.98	0.46
1:D:231:ILE:HG12	1:D:266:CYS:HB2	1.98	0.45
1:B:146:GLU:HB2	1:B:226:PHE:CZ	2.52	0.45
1:D:28:THR:C	1:D:30:TRP:H	2.24	0.45
1:C:107:THR:O	1:C:140:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:GLY:HA3	1:D:411:LYS:HE3	1.98	0.45
1:C:225:HIS:HB2	1:D:225:HIS:HB2	1.99	0.45
1:C:231:ILE:HG12	1:C:266:CYS:HB2	1.99	0.45
1:A:205:THR:HA	1:B:220:CYS:HA	1.99	0.45
1:C:104:PHE:CZ	1:C:251:CYS:HB3	2.52	0.45
1:A:146:GLU:HB2	1:A:226:PHE:CE1	2.52	0.44
1:B:144:ASP:HB2	1:B:159:VAL:HB	1.99	0.44
1:D:25:GLN:HE22	1:D:46:ASP:H	1.66	0.44
1:A:43:GLN:O	1:A:292:SER:OG	2.34	0.43
1:C:146:GLU:HB2	1:C:226:PHE:CZ	2.54	0.43
1:C:263:PHE:HA	1:C:266:CYS:HB3	2.00	0.43
1:D:43:GLN:H	1:D:43:GLN:CD	2.26	0.43
1:D:154:LEU:HD12	1:D:162:PHE:HE2	1.83	0.43
1:A:179:ASN:HD22	1:A:179:ASN:N	2.09	0.43
1:B:255:CYS:O	1:B:282:HIS:HA	2.18	0.43
1:A:118:LEU:HD21	1:A:384:LEU:HD22	2.01	0.42
1:B:104:PHE:CZ	1:B:251:CYS:HB3	2.54	0.42
1:B:424:LYS:HA	1:B:425:PRO:HD3	1.88	0.42
1:C:203:GLN:HB3	1:C:272:LYS:HE2	2.01	0.42
1:C:347:GLN:O	1:C:351:PHE:HD1	2.02	0.42
1:D:239:PHE:HB3	1:D:242:VAL:HB	2.02	0.42
1:D:300:ASP:O	1:D:301:ASP:HB3	2.19	0.42
1:A:217:ASP:HB3	1:B:207:SER:HB2	2.01	0.42
1:A:231:ILE:HG12	1:A:266:CYS:HB2	2.01	0.42
1:D:216:ASN:C	1:D:216:ASN:HD22	2.28	0.41
1:D:291:GLY:O	1:D:294:THR:HG22	2.20	0.41
1:B:26:VAL:O	1:B:32:VAL:HA	2.20	0.41
1:C:82:GLY:O	1:C:284:ARG:HD2	2.21	0.41
1:A:318:ILE:O	1:A:322:ALA:HB3	2.21	0.41
1:C:35:GLY:O	1:C:43:GLN:HB2	2.21	0.41
1:A:253:ILE:HB	1:A:280:LEU:HD23	2.01	0.40
1:A:422:ALA:HA	1:A:423:PRO:HD3	1.93	0.40
1:B:339:ASN:HA	1:B:340:PRO:HD3	1.92	0.40
1:D:51:ILE:HG21	1:D:58:PRO:HD3	2.03	0.40
1:A:27:VAL:HG21	1:A:50:LEU:HD11	2.04	0.40
1:A:146:GLU:HB2	1:A:226:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

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	
1	A	406/438 (93%)	396 (98%)	10 (2%)	0	100	100
1	B	401/438 (92%)	387 (96%)	13 (3%)	1 (0%)	43	76
1	C	401/438 (92%)	387 (96%)	14 (4%)	0	100	100
1	D	408/438 (93%)	396 (97%)	11 (3%)	1 (0%)	43	76
All	All	1616/1752 (92%)	1566 (97%)	48 (3%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	ASP
1	D	29	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	
1	A	361/391 (92%)	349 (97%)	12 (3%)	33	67
1	B	356/391 (91%)	347 (98%)	9 (2%)	42	72
1	C	356/391 (91%)	348 (98%)	8 (2%)	45	74
1	D	363/391 (93%)	348 (96%)	15 (4%)	27	61
All	All	1436/1564 (92%)	1392 (97%)	44 (3%)	35	68

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	43	GLN
1	A	60	ASN
1	A	149	LEU
1	A	151	LYS
1	A	179	ASN
1	A	290	GLN
1	A	294	THR
1	A	359	LEU
1	A	371	LEU
1	A	403	LEU
1	A	421	VAL
1	B	49	LYS
1	B	62	GLU
1	B	68	LYS
1	B	149	LEU
1	B	272	LYS
1	B	302	THR
1	B	349	LEU
1	B	421	VAL
1	B	424	LYS
1	C	23	LYS
1	C	60	ASN
1	C	149	LEU
1	C	328	VAL
1	C	349	LEU
1	C	371	LEU
1	C	417	LYS
1	C	421	VAL
1	D	28	THR
1	D	43	GLN
1	D	44	ASN
1	D	50	LEU
1	D	62	GLU
1	D	149	LEU
1	D	154	LEU
1	D	216	ASN
1	D	241	ASN
1	D	289	LEU
1	D	290	GLN
1	D	303	THR
1	D	328	VAL
1	D	360	LYS

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Mol	Chain	Res	Type
1	D	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	ASN
1	A	53	GLN
1	A	60	ASN
1	A	99	GLN
1	A	131	GLN
1	A	179	ASN
1	A	313	GLN
1	A	385	GLN
1	B	53	GLN
1	B	99	GLN
1	B	333	HIS
1	B	339	ASN
1	B	385	GLN
1	C	43	GLN
1	C	44	ASN
1	C	60	ASN
1	C	187	GLN
1	C	313	GLN
1	C	339	ASN
1	C	385	GLN
1	D	25	GLN
1	D	53	GLN
1	D	120	HIS
1	D	216	ASN
1	D	241	ASN
1	D	290	GLN
1	D	313	GLN
1	D	333	HIS
1	D	385	GLN

5.3.3 RNA ⓘ

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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LTN	A	500	-	16,16,16	1.40	4 (25%)	22,22,22	0.76	1 (4%)
3	SO4	D	440	-	4,4,4	0.24	0	6,6,6	0.10	0
2	LTN	D	800	-	16,16,16	1.40	4 (25%)	22,22,22	0.76	0
3	SO4	C	439	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	C	440	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	439	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	439	-	4,4,4	0.24	0	6,6,6	0.07	0
2	LTN	B	700	-	16,16,16	1.41	4 (25%)	22,22,22	0.79	1 (4%)
3	SO4	B	440	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	A	440	-	4,4,4	0.23	0	6,6,6	0.09	0
2	LTN	C	600	-	16,16,16	1.39	3 (18%)	22,22,22	0.77	1 (4%)
3	SO4	A	441	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	439	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	441	-	4,4,4	0.26	0	6,6,6	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LTN	A	500	-	-	1/8/8/8	0/2/2/2
2	LTN	D	800	-	-	1/8/8/8	0/2/2/2
2	LTN	B	700	-	-	1/8/8/8	0/2/2/2
2	LTN	C	600	-	-	1/8/8/8	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	LTN	CD2-CG	-2.86	1.39	1.44
2	A	500	LTN	CD2-CG	-2.86	1.39	1.44
2	C	600	LTN	CD2-CG	-2.83	1.39	1.44
2	D	800	LTN	CD2-CG	-2.78	1.39	1.44
2	C	600	LTN	CE2-NE1	-2.73	1.33	1.37
2	B	700	LTN	CE2-NE1	-2.71	1.33	1.37
2	A	500	LTN	CE2-NE1	-2.70	1.33	1.37
2	D	800	LTN	CE2-NE1	-2.70	1.33	1.37
2	D	800	LTN	CD1-CG	-2.22	1.33	1.36
2	B	700	LTN	CD1-CG	-2.17	1.33	1.36
2	B	700	LTN	CD1-NE1	-2.16	1.33	1.37
2	A	500	LTN	CD1-CG	-2.13	1.33	1.36
2	A	500	LTN	CD1-NE1	-2.09	1.33	1.37
2	C	600	LTN	CD1-CG	-2.09	1.33	1.36
2	D	800	LTN	CD1-NE1	-2.07	1.33	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	LTN	CZ2-CE2-CD2	-2.07	120.19	122.19
2	C	600	LTN	CZ2-CE2-CD2	-2.03	120.22	122.19
2	A	500	LTN	CZ2-CE2-CD2	-2.01	120.25	122.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	LTN	NH3-CA-CB-CG
2	B	700	LTN	NH3-CA-CB-CG
2	D	800	LTN	NH3-CA-CB-CG
2	C	600	LTN	NH3-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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	408/438 (93%)	0.48	28 (6%) 23 12	63, 72, 96, 106	0
1	B	403/438 (92%)	0.75	35 (8%) 16 8	49, 83, 120, 135	0
1	C	403/438 (92%)	0.62	36 (8%) 15 8	61, 74, 112, 122	0
1	D	410/438 (93%)	0.71	34 (8%) 17 9	70, 83, 100, 109	0
All	All	1624/1752 (92%)	0.64	133 (8%) 17 9	49, 78, 106, 135	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ALA	6.6
1	B	294	THR	6.0
1	C	294	THR	5.9
1	C	296	MET	5.2
1	C	298	ALA	4.9
1	C	293	THR	4.9
1	B	26	VAL	4.8
1	C	295	LYS	4.6
1	A	22	VAL	4.3
1	A	299	SER	4.3
1	A	293	THR	4.2
1	C	297	SER	4.1
1	B	293	THR	4.1
1	C	42	ALA	4.0
1	C	23	LYS	3.9
1	D	22	VAL	3.9
1	C	425	PRO	3.8
1	C	40	GLY	3.7
1	B	425	PRO	3.7
1	D	21	ASP	3.6
1	B	302	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	241	ASN	3.6
1	B	296	MET	3.6
1	A	425	PRO	3.6
1	C	292	SER	3.6
1	A	37	ASP	3.5
1	A	295	LYS	3.5
1	A	294	THR	3.5
1	D	425	PRO	3.5
1	C	39	GLN	3.4
1	A	298	ALA	3.4
1	D	295	LYS	3.3
1	A	18	LYS	3.3
1	B	27	VAL	3.2
1	B	24	GLU	3.2
1	C	272	LYS	3.2
1	C	299	SER	3.2
1	D	308	THR	3.1
1	D	294	THR	3.1
1	B	37	ASP	3.1
1	C	34	GLY	3.0
1	D	43	GLN	3.0
1	C	26	VAL	3.0
1	A	31	ASP	3.0
1	D	176	ASP	3.0
1	C	152	HIS	3.0
1	B	297	SER	2.9
1	C	45	ILE	2.9
1	B	31	ASP	2.8
1	C	36	VAL	2.8
1	D	300	ASP	2.8
1	B	36	VAL	2.8
1	B	42	ALA	2.7
1	B	271	ASP	2.7
1	D	37	ASP	2.7
1	B	152	HIS	2.7
1	C	25	GLN	2.7
1	B	33	GLU	2.7
1	A	264	ARG	2.7
1	B	23	LYS	2.7
1	B	329	SER	2.7
1	C	41	ARG	2.6
1	C	38	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	155	THR	2.6
1	A	152	HIS	2.6
1	C	33	GLU	2.6
1	B	292	SER	2.6
1	D	16	GLU	2.6
1	C	32	VAL	2.6
1	A	424	LYS	2.6
1	C	35	GLY	2.5
1	B	295	LYS	2.5
1	D	18	LYS	2.5
1	D	28	THR	2.5
1	A	34	GLY	2.4
1	D	74	GLU	2.4
1	A	258	ASP	2.4
1	B	311	PRO	2.4
1	A	21	ASP	2.4
1	D	421	VAL	2.4
1	C	291	GLY	2.4
1	B	114	ASP	2.4
1	C	37	ASP	2.4
1	B	400	GLU	2.4
1	D	297	SER	2.4
1	D	152	HIS	2.3
1	B	418	GLU	2.3
1	D	301	ASP	2.3
1	D	420	LEU	2.3
1	B	316	LYS	2.3
1	A	19	SER	2.3
1	C	117	HIS	2.3
1	A	33	GLU	2.3
1	B	300	ASP	2.3
1	A	297	SER	2.3
1	A	69	GLN	2.3
1	A	271	ASP	2.3
1	C	300	ASP	2.3
1	C	24	GLU	2.2
1	D	422	ALA	2.2
1	C	400	GLU	2.2
1	D	296	MET	2.2
1	B	274	LYS	2.2
1	B	319	ASN	2.2
1	C	62	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLY	2.2
1	D	72	GLY	2.2
1	A	300	ASP	2.2
1	B	117	HIS	2.2
1	D	292	SER	2.2
1	D	17	LEU	2.2
1	C	416	GLU	2.2
1	A	20	THR	2.1
1	D	114	ASP	2.1
1	D	293	THR	2.1
1	A	290	GLN	2.1
1	C	69	GLN	2.1
1	D	61	GLU	2.1
1	A	292	SER	2.1
1	A	61	GLU	2.1
1	D	75	PRO	2.1
1	C	115	SER	2.0
1	D	44	ASN	2.0
1	A	301	ASP	2.0
1	B	46	ASP	2.0
1	B	308	THR	2.0
1	D	62	GLU	2.0
1	D	382	GLU	2.0
1	A	36	VAL	2.0
1	D	271	ASP	2.0
1	B	187	GLN	2.0
1	B	62	GLU	2.0
1	D	132	GLU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	440	5/5	0.71	0.24	100,100,100,100	5
3	SO4	B	441	5/5	0.72	0.16	102,102,102,102	5
3	SO4	A	439	5/5	0.81	0.11	102,102,102,102	5
3	SO4	B	440	5/5	0.86	0.12	82,82,82,82	5
3	SO4	B	439	5/5	0.87	0.09	89,89,89,89	5
3	SO4	D	439	5/5	0.89	0.10	80,80,80,80	5
3	SO4	A	440	5/5	0.92	0.10	81,81,81,81	5
3	SO4	A	441	5/5	0.93	0.09	78,78,78,78	5
2	LTN	D	800	15/15	0.93	0.11	73,73,73,73	0
2	LTN	A	500	15/15	0.94	0.12	68,68,68,68	0
2	LTN	B	700	15/15	0.95	0.10	78,79,79,79	0
3	SO4	C	439	5/5	0.95	0.08	64,64,64,64	5
2	LTN	C	600	15/15	0.96	0.10	74,74,75,75	0
3	SO4	D	440	5/5	0.96	0.11	59,59,59,59	5

6.5 Other polymers

There are no such residues in this entry.