



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:19 AM UTC

PDB ID : 3KT6 / pdb_00003kt6
Title : Crystal structure of *S. cerevisiae* tryptophanyl-tRNA synthetase in complex with Trp
Authors : Zhou, M.; Dong, X.; Zhong, C.; Shen, N.; Ding, J.
Deposited on : 2009-11-24
Resolution : 2.80 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

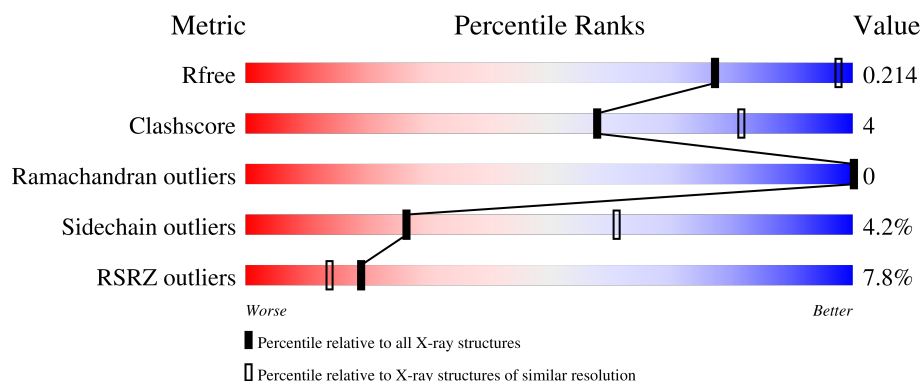
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

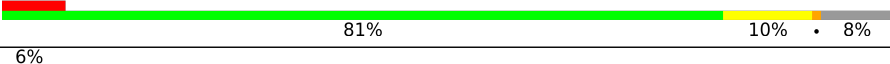
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	B	438	
1	C	438	
1	D	438	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13292 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	409	Total	C	N	O	S	0	0	0
			3295	2124	546	612	13			
1	B	404	Total	C	N	O	S	0	0	0
			3257	2101	540	603	13			
1	C	404	Total	C	N	O	S	0	0	0
			3257	2101	540	603	13			
1	D	409	Total	C	N	O	S	0	0	0
			3295	2124	546	612	13			

There are 24 discrepancies between the modelled and reference sequences:

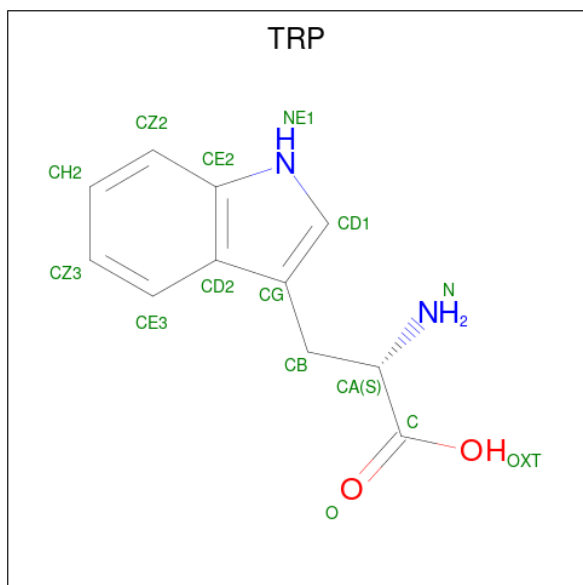
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	HIS	-	expression tag	UNP Q12109
A	434	HIS	-	expression tag	UNP Q12109
A	435	HIS	-	expression tag	UNP Q12109
A	436	HIS	-	expression tag	UNP Q12109
A	437	HIS	-	expression tag	UNP Q12109
A	438	HIS	-	expression tag	UNP Q12109
B	433	HIS	-	expression tag	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 TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



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

- 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	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	C	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	25	Total	O	0	0
			25	25		

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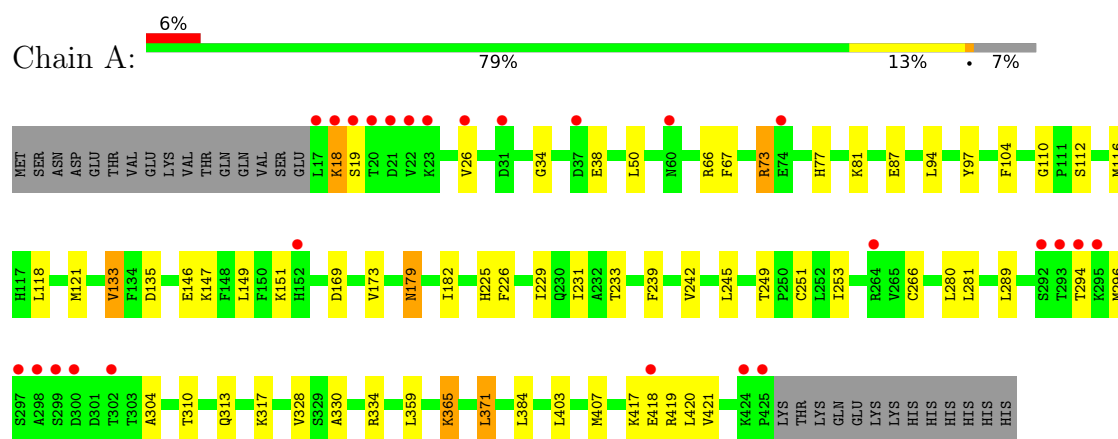
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total	O	0	0
			20	20		
4	C	17	Total	O	0	0
			17	17		
4	D	11	Total	O	0	0
			11	11		

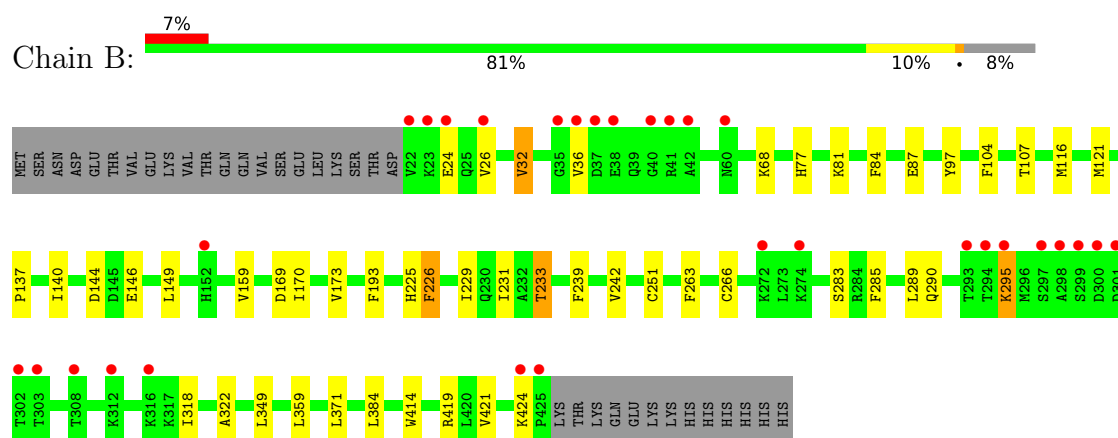
3 Residue-property plots [i](#)

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.

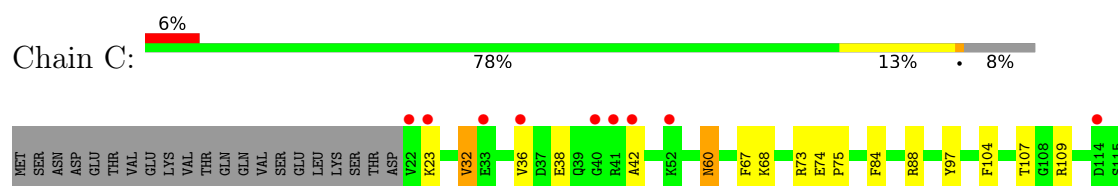
- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

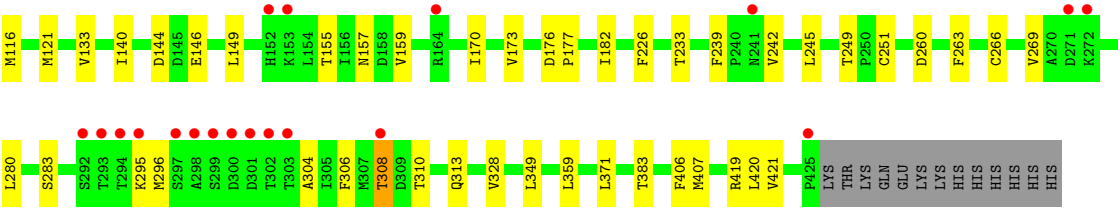


- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

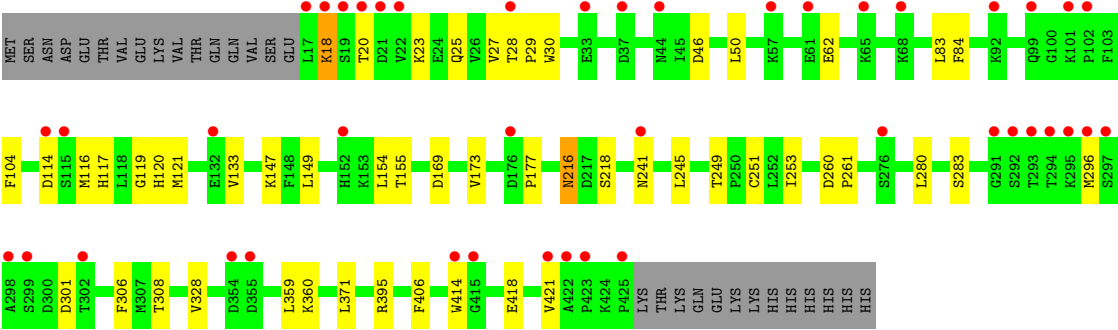
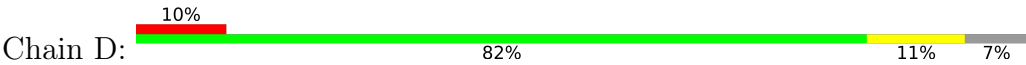


- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic





● 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	252.66Å 252.66Å 111.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.75 – 2.80 47.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.75-2.80) 99.4 (47.75-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.247 0.213 , 0.214	Depositor DCC
R_{free} test set	4964 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

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	0.44	1/3377 (0.0%)	0.77	1/4557 (0.0%)
1	B	0.42	0/3339	0.77	1/4506 (0.0%)
1	C	0.43	0/3339	0.78	0/4506
1	D	0.44	0/3377	0.79	0/4557
All	All	0.43	1/13432 (0.0%)	0.78	2/18126 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLU	CD-OE1	5.31	1.35	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	PHE	N-CA-C	5.48	117.97	111.33
1	A	34	GLY	N-CA-C	5.15	119.36	112.77

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	3295	0	3258	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3257	0	3218	24	0
1	C	3257	0	3218	32	0
1	D	3295	0	3258	26	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
3	A	20	0	0	2	0
3	B	10	0	0	0	0
3	C	15	0	0	2	0
3	D	10	0	0	1	0
4	A	25	0	0	1	0
4	B	20	0	0	0	0
4	C	17	0	0	0	0
4	D	11	0	0	1	0
All	All	13292	0	12988	118	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 4.

All (118) 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:B:116:MET:HE1	1:B:170:ILE:HG13	1.57	0.85
1:B:116:MET:HE3	1:B:169:ASP:HB2	1.58	0.84
1:A:310:THR:H	1:A:313:GLN:HE21	1.33	0.75
1:B:116:MET:HE3	1:B:169:ASP:CB	2.22	0.68
1:C:310:THR:H	1:C:313:GLN:HE21	1.41	0.67
1:C:121:MET:HE1	1:C:173:VAL:HG22	1.77	0.67
1:A:418:GLU:H	1:A:418:GLU:CD	2.01	0.67
1:A:179:ASN:H	1:A:179:ASN:HD22	1.43	0.65
1:A:310:THR:H	1:A:313:GLN:NE2	1.95	0.64
1:C:116:MET:HE1	1:C:170:ILE:HG13	1.80	0.62
1:A:330:ALA:O	1:A:334:ARG:HG2	1.99	0.62
1:B:318:ILE:HD11	1:B:384:LEU:HD12	1.82	0.62
1:C:88:ARG:NH2	1:C:260:ASP:OD1	2.34	0.59
1:C:23:LYS:HB3	1:C:36:VAL:HG22	1.85	0.59
1:D:121:MET:HE1	1:D:173:VAL:HG22	1.86	0.58
1:B:285:PHE:HB3	1:B:295:LYS:HB3	1.86	0.58
1:A:77:HIS:HB2	1:A:81:LYS:HE3	1.87	0.57
1:A:253:ILE:HB	1:A:280:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG21	1:D:23:LYS:HD3	1.86	0.56
1:A:146:GLU:HB2	1:A:226:PHE:CZ	2.41	0.56
1:C:239:PHE:HB3	1:C:242:VAL:HB	1.87	0.55
1:C:109:ARG:HG2	1:C:116:MET:HE2	1.88	0.54
1:D:18:LYS:H	1:D:18:LYS:HD3	1.71	0.54
1:C:60:ASN:C	1:C:60:ASN:HD22	2.14	0.53
1:C:310:THR:H	1:C:313:GLN:NE2	2.05	0.53
1:B:97:TYR:O	1:B:419:ARG:NH2	2.35	0.51
1:D:117:HIS:CE1	1:D:296:MET:HG2	2.45	0.51
1:A:66:ARG:HG2	1:A:94:LEU:HD13	1.92	0.51
1:C:32:VAL:HG11	1:C:295:LYS:HD3	1.91	0.51
1:D:253:ILE:HB	1:D:280:LEU:HD23	1.91	0.51
1:A:67:PHE:HZ	1:A:133:VAL:HG11	1.76	0.51
1:A:121:MET:HE1	1:A:173:VAL:HG22	1.92	0.51
1:D:418:GLU:H	1:D:418:GLU:CD	2.19	0.51
1:C:67:PHE:HZ	1:C:133:VAL:HG11	1.75	0.51
1:C:104:PHE:CZ	1:C:251:CYS:HB3	2.46	0.51
1:A:110:GLY:HA3	1:A:147:LYS:HE3	1.91	0.50
1:A:239:PHE:HB3	1:A:242:VAL:HB	1.92	0.50
1:A:112:SER:HB3	1:A:147:LYS:HD2	1.93	0.49
1:D:25:GLN:HE22	1:D:46:ASP:H	1.59	0.49
1:A:87:GLU:HB3	1:A:281:LEU:HD23	1.94	0.49
1:D:260:ASP:N	1:D:261:PRO:HD2	2.26	0.49
1:A:334:ARG:HG3	4:A:521:HOH:O	2.12	0.49
1:C:245:LEU:HD13	1:C:249:THR:HG21	1.94	0.49
1:C:67:PHE:CZ	1:C:133:VAL:HG11	2.48	0.48
1:A:104:PHE:CZ	1:A:251:CYS:HB3	2.49	0.48
1:D:216:ASN:C	1:D:216:ASN:HD22	2.21	0.48
1:B:116:MET:CE	1:B:169:ASP:HB2	2.39	0.48
1:C:36:VAL:HG12	1:C:42:ALA:HA	1.94	0.48
1:D:301:ASP:HA	1:D:306:PHE:HE2	1.79	0.47
1:B:32:VAL:HG11	1:B:295:LYS:HG2	1.97	0.47
1:B:239:PHE:HB3	1:B:242:VAL:HB	1.97	0.47
1:C:155:THR:HG22	1:C:157:ASN:H	1.78	0.47
1:B:107:THR:O	1:B:140:ILE:HA	2.15	0.47
1:C:88:ARG:HH21	1:C:260:ASP:CG	2.22	0.47
1:D:104:PHE:CZ	1:D:251:CYS:HB3	2.50	0.47
1:D:84:PHE:CE2	1:D:283:SER:HB3	2.50	0.46
1:B:121:MET:HE1	1:B:173:VAL:HG22	1.98	0.46
1:B:137:PRO:HD3	1:B:414:TRP:CG	2.50	0.46
1:B:146:GLU:HB2	1:B:226:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD21	1:D:414:TRP:HZ2	1.81	0.46
1:C:84:PHE:CZ	1:C:283:SER:HB3	2.51	0.46
1:D:84:PHE:CZ	1:D:283:SER:HB3	2.51	0.46
1:B:77:HIS:HB2	1:B:81:LYS:HE3	1.97	0.46
1:A:118:LEU:HD21	1:A:384:LEU:HD22	1.97	0.45
1:A:116:MET:HE2	1:A:169:ASP:HB3	1.98	0.45
1:A:135:ASP:OD2	1:A:417:LYS:HG2	2.16	0.45
1:D:28:THR:HG22	1:D:30:TRP:H	1.82	0.45
1:C:306:PHE:C	1:C:308:THR:H	2.24	0.45
1:C:146:GLU:HB2	1:C:226:PHE:CZ	2.52	0.44
1:C:263:PHE:HA	1:C:266:CYS:HB3	1.99	0.44
1:B:144:ASP:HB2	1:B:159:VAL:HB	2.00	0.44
1:A:245:LEU:HD13	1:A:249:THR:HG21	1.99	0.44
1:C:73:ARG:NE	3:C:602:SO4:O1	2.39	0.44
1:C:176:ASP:OD1	1:C:177:PRO:HD2	2.17	0.44
1:D:245:LEU:HD13	1:D:249:THR:HG21	2.00	0.44
1:B:84:PHE:CZ	1:B:283:SER:HB3	2.53	0.44
1:B:104:PHE:CZ	1:B:251:CYS:HB3	2.53	0.44
1:D:119:GLY:H	1:D:296:MET:HE2	1.83	0.44
1:C:182:ILE:O	1:C:407:MET:HA	2.18	0.43
1:A:179:ASN:HD22	1:A:179:ASN:N	2.07	0.43
1:A:225:HIS:HB2	1:B:225:HIS:HB2	2.00	0.43
1:C:177:PRO:HD3	1:C:406:PHE:CZ	2.53	0.43
1:C:74:GLU:HG2	1:C:75:PRO:HD2	2.00	0.43
1:D:116:MET:HE2	1:D:120:HIS:HB3	2.00	0.43
1:A:73:ARG:CG	1:A:73:ARG:HH21	2.31	0.43
1:A:182:ILE:O	1:A:407:MET:HA	2.18	0.43
1:D:27:VAL:HG21	1:D:50:LEU:HD11	2.01	0.43
1:A:67:PHE:CZ	1:A:133:VAL:HG11	2.53	0.43
1:A:365:LYS:HB3	1:A:371:LEU:HB2	2.01	0.43
1:C:144:ASP:HB2	1:C:159:VAL:HB	2.01	0.43
1:B:231:ILE:HG12	1:B:266:CYS:HB2	2.00	0.42
1:C:97:TYR:O	1:C:419:ARG:NH2	2.33	0.42
1:C:155:THR:HG23	3:C:603:SO4:O4	2.19	0.42
1:D:121:MET:CE	1:D:173:VAL:HG22	2.48	0.42
1:D:169:ASP:OD1	1:D:395:ARG:NE	2.49	0.42
1:B:193:PHE:CE1	1:B:233:THR:HG22	2.55	0.42
1:B:289:LEU:O	1:B:322:ALA:HA	2.20	0.42
1:D:241:ASN:ND2	4:D:808:HOH:O	2.50	0.42
1:A:73:ARG:CD	3:A:502:SO4:O3	2.68	0.42
1:B:229:ILE:O	1:B:233:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:MET:CE	1:A:173:VAL:HG22	2.50	0.41
1:D:216:ASN:HD22	1:D:218:SER:H	1.68	0.41
1:D:155:THR:HB	3:D:802:SO4:O3	2.20	0.41
1:A:97:TYR:O	1:A:419:ARG:NH2	2.27	0.41
1:A:231:ILE:HG12	1:A:266:CYS:HB2	2.03	0.41
1:A:229:ILE:O	1:A:233:THR:HG23	2.21	0.41
1:B:26:VAL:O	1:B:32:VAL:HA	2.20	0.41
1:D:28:THR:HG23	1:D:29:PRO:HD2	2.03	0.41
1:C:104:PHE:CE2	1:C:251:CYS:HB3	2.55	0.41
1:A:289:LEU:HD21	1:A:317:LYS:HB3	2.03	0.41
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.79	0.41
1:A:296:MET:HE2	1:A:304:ALA:HA	2.02	0.40
1:B:263:PHE:HA	1:B:266:CYS:HB3	2.04	0.40
1:C:107:THR:O	1:C:140:ILE:HA	2.21	0.40
1:A:18:LYS:CE	1:A:19:SER:H	2.35	0.40
1:C:296:MET:HE2	1:C:304:ALA:HA	2.03	0.40
1:D:177:PRO:HD3	1:D:406:PHE:CZ	2.57	0.40
1:A:73:ARG:HD2	3:A:502:SO4:O3	2.21	0.40

There are no symmetry-related clashes.

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	407/438 (93%)	397 (98%)	10 (2%)	0	100	100
1	B	402/438 (92%)	389 (97%)	13 (3%)	0	100	100
1	C	402/438 (92%)	391 (97%)	11 (3%)	0	100	100
1	D	407/438 (93%)	395 (97%)	12 (3%)	0	100	100
All	All	1618/1752 (92%)	1572 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	362/391 (93%)	347 (96%)	15 (4%)	27	62
1	B	357/391 (91%)	343 (96%)	14 (4%)	28	64
1	C	357/391 (91%)	341 (96%)	16 (4%)	24	58
1	D	362/391 (93%)	346 (96%)	16 (4%)	25	59
All	All	1438/1564 (92%)	1377 (96%)	61 (4%)	26	61

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	50	LEU
1	A	73	ARG
1	A	133	VAL
1	A	149	LEU
1	A	151	LYS
1	A	179	ASN
1	A	294	THR
1	A	328	VAL
1	A	359	LEU
1	A	365	LYS
1	A	371	LEU
1	A	403	LEU
1	A	420	LEU
1	A	421	VAL
1	B	24	GLU
1	B	32	VAL
1	B	36	VAL
1	B	68	LYS
1	B	87	GLU
1	B	149	LEU
1	B	233	THR
1	B	290	GLN
1	B	295	LYS

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Mol	Chain	Res	Type
1	B	349	LEU
1	B	359	LEU
1	B	371	LEU
1	B	421	VAL
1	B	424	LYS
1	C	32	VAL
1	C	38	GLU
1	C	60	ASN
1	C	68	LYS
1	C	149	LEU
1	C	233	THR
1	C	269	VAL
1	C	280	LEU
1	C	308	THR
1	C	328	VAL
1	C	349	LEU
1	C	359	LEU
1	C	371	LEU
1	C	383	THR
1	C	420	LEU
1	C	421	VAL
1	D	18	LYS
1	D	20	THR
1	D	62	GLU
1	D	83	LEU
1	D	114	ASP
1	D	133	VAL
1	D	147	LYS
1	D	149	LEU
1	D	154	LEU
1	D	216	ASN
1	D	308	THR
1	D	328	VAL
1	D	359	LEU
1	D	360	LYS
1	D	371	LEU
1	D	421	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	131	GLN
1	A	179	ASN
1	A	313	GLN
1	A	385	GLN
1	B	43	GLN
1	B	99	GLN
1	B	187	GLN
1	B	339	ASN
1	B	385	GLN
1	C	60	ASN
1	C	290	GLN
1	C	313	GLN
1	C	339	ASN
1	C	385	GLN
1	D	25	GLN
1	D	53	GLN
1	D	99	GLN
1	D	216	ASN
1	D	230	GLN
1	D	259	GLN
1	D	290	GLN
1	D	313	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
3	SO4	C	603	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	A	703	-	4,4,4	0.37	0	6,6,6	0.15	0
2	TRP	C	600	-	15,16,16	0.77	1 (6%)	18,22,22	0.76	1 (5%)
3	SO4	B	701	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	A	502	-	4,4,4	0.42	0	6,6,6	0.09	0
3	SO4	B	702	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	C	601	-	4,4,4	0.27	0	6,6,6	0.13	0
2	TRP	A	500	-	15,16,16	0.73	1 (6%)	18,22,22	0.79	1 (5%)
3	SO4	C	602	-	4,4,4	0.24	0	6,6,6	0.19	0
2	TRP	D	800	-	15,16,16	0.74	1 (6%)	18,22,22	0.72	1 (5%)
2	TRP	B	700	-	15,16,16	0.74	1 (6%)	18,22,22	0.74	1 (5%)
3	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	D	801	-	4,4,4	0.33	0	6,6,6	0.14	0
3	SO4	D	802	-	4,4,4	0.32	0	6,6,6	0.24	0
3	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.23	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	TRP	C	600	-	-	0/8/8/8	0/2/2/2
2	TRP	D	800	-	-	0/8/8/8	0/2/2/2
2	TRP	B	700	-	-	0/8/8/8	0/2/2/2
2	TRP	A	500	-	-	0/8/8/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	TRP	OXT-C	-2.25	1.23	1.30
2	A	500	TRP	OXT-C	-2.23	1.23	1.30
2	B	700	TRP	OXT-C	-2.22	1.23	1.30
2	C	600	TRP	OXT-C	-2.18	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	TRP	OXT-C-O	-2.93	117.43	124.08
2	C	600	TRP	OXT-C-O	-2.68	118.00	124.08
2	B	700	TRP	OXT-C-O	-2.67	118.03	124.08
2	D	800	TRP	OXT-C-O	-2.57	118.26	124.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	SO4	1	0
3	A	502	SO4	2	0
3	C	602	SO4	1	0
3	D	802	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	409/438 (93%)	0.20	26 (6%) 25 18	42, 58, 98, 141	0
1	B	404/438 (92%)	0.43	30 (7%) 20 15	35, 64, 104, 156	0
1	C	404/438 (92%)	0.26	28 (6%) 23 16	36, 59, 110, 151	0
1	D	409/438 (93%)	0.79	43 (10%) 11 8	49, 71, 107, 138	0
All	All	1626/1752 (92%)	0.42	127 (7%) 19 14	35, 63, 105, 156	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	LYS	8.2
1	D	298	ALA	7.3
1	A	22	VAL	7.2
1	D	21	ASP	6.3
1	C	22	VAL	6.0
1	B	22	VAL	5.6
1	C	425	PRO	5.6
1	A	298	ALA	5.3
1	C	298	ALA	5.3
1	D	241	ASN	5.2
1	D	22	VAL	4.9
1	A	425	PRO	4.8
1	B	298	ALA	4.8
1	D	20	THR	4.8
1	D	293	THR	4.7
1	B	425	PRO	4.5
1	D	425	PRO	4.5
1	D	17	LEU	4.5
1	C	294	THR	4.4
1	D	294	THR	4.4
1	A	299	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	299	SER	4.2
1	A	18	LYS	4.1
1	B	302	THR	4.0
1	A	21	ASP	4.0
1	D	102	PRO	4.0
1	D	297	SER	3.9
1	B	41	ARG	3.8
1	C	42	ALA	3.8
1	D	292	SER	3.8
1	D	421	VAL	3.7
1	B	152	HIS	3.7
1	C	152	HIS	3.7
1	B	294	THR	3.6
1	D	423	PRO	3.5
1	C	293	THR	3.4
1	C	40	GLY	3.3
1	B	316	LYS	3.3
1	B	26	VAL	3.3
1	A	17	LEU	3.2
1	C	300	ASP	3.1
1	B	274	LYS	3.1
1	C	297	SER	3.1
1	D	57	LYS	3.1
1	A	293	THR	3.1
1	B	303	THR	3.1
1	D	68	LYS	3.0
1	B	40	GLY	3.0
1	C	301	ASP	3.0
1	C	36	VAL	3.0
1	D	28	THR	2.9
1	C	292	SER	2.9
1	B	293	THR	2.9
1	B	295	LYS	2.9
1	D	115	SER	2.9
1	A	294	THR	2.9
1	A	19	SER	2.9
1	A	292	SER	2.9
1	C	295	LYS	2.8
1	A	297	SER	2.8
1	C	23	LYS	2.8
1	C	272	LYS	2.8
1	A	264	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	2.8
1	D	414	TRP	2.8
1	A	152	HIS	2.7
1	A	60	ASN	2.7
1	A	37	ASP	2.7
1	B	42	ALA	2.7
1	C	241	ASN	2.7
1	B	299	SER	2.7
1	A	23	LYS	2.6
1	C	303	THR	2.6
1	D	295	LYS	2.6
1	A	20	THR	2.6
1	D	422	ALA	2.6
1	D	99	GLN	2.6
1	D	291	GLY	2.5
1	D	114	ASP	2.5
1	B	312	LYS	2.5
1	D	37	ASP	2.5
1	D	296	MET	2.5
1	A	31	ASP	2.5
1	B	308	THR	2.5
1	C	302	THR	2.5
1	D	176	ASP	2.4
1	D	299	SER	2.4
1	A	295	LYS	2.4
1	C	153	LYS	2.4
1	A	26	VAL	2.4
1	C	308	THR	2.4
1	C	164	ARG	2.3
1	D	65	LYS	2.3
1	B	300	ASP	2.3
1	C	114	ASP	2.3
1	A	418	GLU	2.3
1	B	35	GLY	2.3
1	B	37	ASP	2.3
1	C	271	ASP	2.3
1	B	60	ASN	2.3
1	D	19	SER	2.3
1	D	415	GLY	2.3
1	A	74	GLU	2.3
1	A	300	ASP	2.3
1	A	424	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	24	GLU	2.2
1	C	33	GLU	2.2
1	D	33	GLU	2.2
1	D	276	SER	2.2
1	D	61	GLU	2.2
1	B	23	LYS	2.2
1	D	92	LYS	2.2
1	C	41	ARG	2.2
1	B	36	VAL	2.2
1	B	272	LYS	2.2
1	B	297	SER	2.2
1	D	132	GLU	2.2
1	B	38	GLU	2.1
1	A	302	THR	2.1
1	D	302	THR	2.1
1	D	355	ASP	2.1
1	B	424	LYS	2.1
1	C	52	LYS	2.0
1	D	44	ASN	2.0
1	D	354	ASP	2.0
1	D	152	HIS	2.0
1	D	101	LYS	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	D	801	5/5	0.81	0.18	90,95,95,95	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	501	5/5	0.85	0.16	89,95,95,95	5
3	SO4	B	701	5/5	0.87	0.12	83,87,87,87	0
3	SO4	A	503	5/5	0.87	0.18	43,56,57,57	5
3	SO4	A	502	5/5	0.88	0.15	45,58,59,60	5
3	SO4	C	601	5/5	0.89	0.18	48,60,62,62	5
3	SO4	B	702	5/5	0.89	0.17	44,56,57,57	5
3	SO4	C	603	5/5	0.90	0.20	45,56,57,57	5
3	SO4	A	703	5/5	0.94	0.17	42,54,56,56	5
2	TRP	D	800	15/15	0.95	0.11	72,72,74,74	0
3	SO4	C	602	5/5	0.95	0.10	38,52,53,53	5
3	SO4	D	802	5/5	0.95	0.15	41,53,55,55	5
2	TRP	B	700	15/15	0.96	0.09	53,54,61,61	0
2	TRP	A	500	15/15	0.97	0.09	56,56,62,62	0
2	TRP	C	600	15/15	0.97	0.08	49,50,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.