



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 12:25 AM UTC

PDB ID : 6WOM / pdb_00006wom
Title : Crystal structure of Aspartyl-tRNA ligase from Elizabethkingia sp.
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-04-24
Resolution : 2.15 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

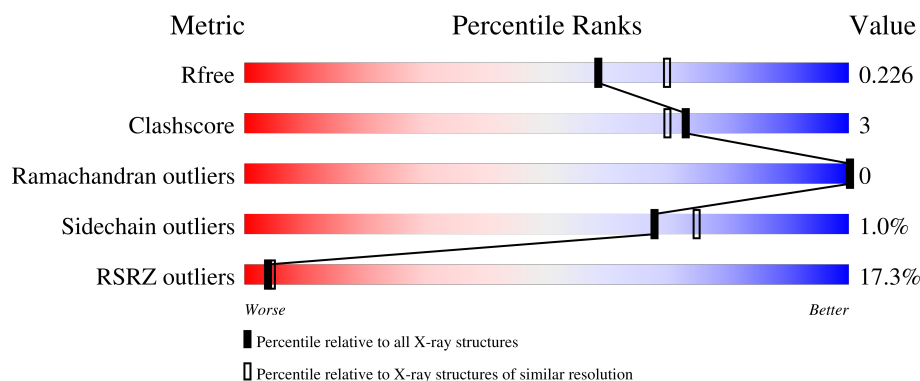
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	592	2% 90% 8% .
1	B	592	2% 92% 6% .
1	C	592	47% 85% 8% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14257 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 Aspartate-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	4	0
			4635	2957	785	873	20			
1	B	583	Total	C	N	O	S	0	4	0
			4622	2948	779	874	21			
1	C	549	Total	C	N	O	S	0	0	0
			3941	2499	680	744	18			

There are 24 discrepancies between the modelled and reference sequences:

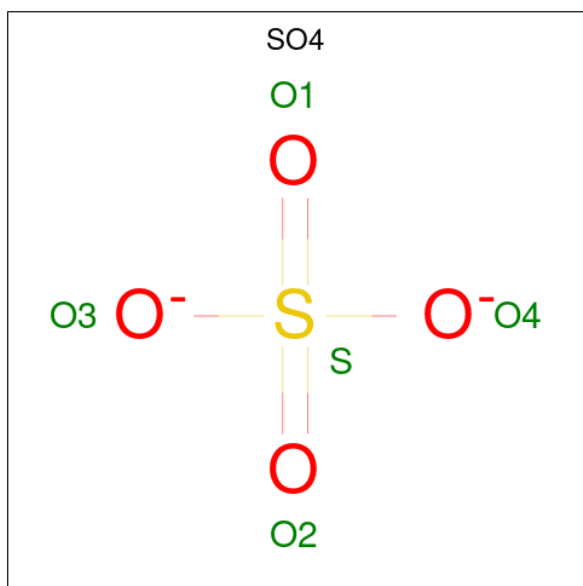
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A1T3DDI2
A	-6	ALA	-	expression tag	UNP A0A1T3DDI2
A	-5	HIS	-	expression tag	UNP A0A1T3DDI2
A	-4	HIS	-	expression tag	UNP A0A1T3DDI2
A	-3	HIS	-	expression tag	UNP A0A1T3DDI2
A	-2	HIS	-	expression tag	UNP A0A1T3DDI2
A	-1	HIS	-	expression tag	UNP A0A1T3DDI2
A	0	HIS	-	expression tag	UNP A0A1T3DDI2
B	-7	MET	-	initiating methionine	UNP A0A1T3DDI2
B	-6	ALA	-	expression tag	UNP A0A1T3DDI2
B	-5	HIS	-	expression tag	UNP A0A1T3DDI2
B	-4	HIS	-	expression tag	UNP A0A1T3DDI2
B	-3	HIS	-	expression tag	UNP A0A1T3DDI2
B	-2	HIS	-	expression tag	UNP A0A1T3DDI2
B	-1	HIS	-	expression tag	UNP A0A1T3DDI2
B	0	HIS	-	expression tag	UNP A0A1T3DDI2
C	-7	MET	-	initiating methionine	UNP A0A1T3DDI2
C	-6	ALA	-	expression tag	UNP A0A1T3DDI2
C	-5	HIS	-	expression tag	UNP A0A1T3DDI2
C	-4	HIS	-	expression tag	UNP A0A1T3DDI2
C	-3	HIS	-	expression tag	UNP A0A1T3DDI2
C	-2	HIS	-	expression tag	UNP A0A1T3DDI2
C	-1	HIS	-	expression tag	UNP A0A1T3DDI2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A1T3DDI2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

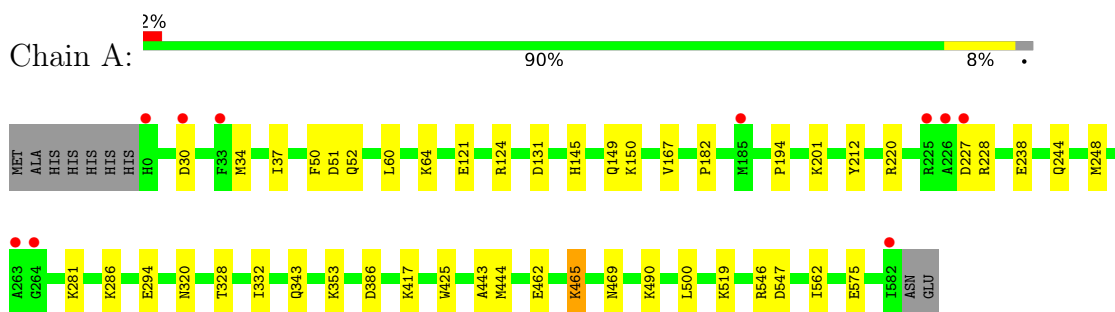
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	537	Total O 544 544	0	7
3	B	447	Total O 450 450	0	3
3	C	54	Total O 55 55	0	1

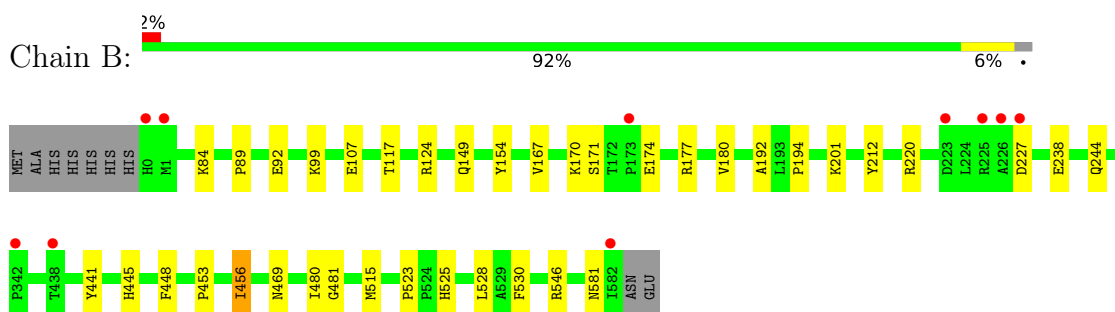
3 Residue-property plots [i](#)

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.

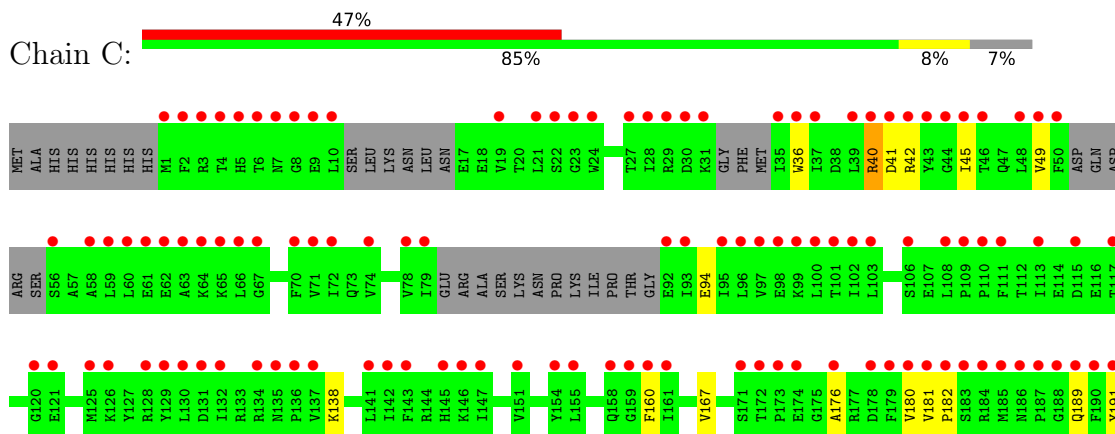
• Molecule 1: Aspartate-tRNA ligase

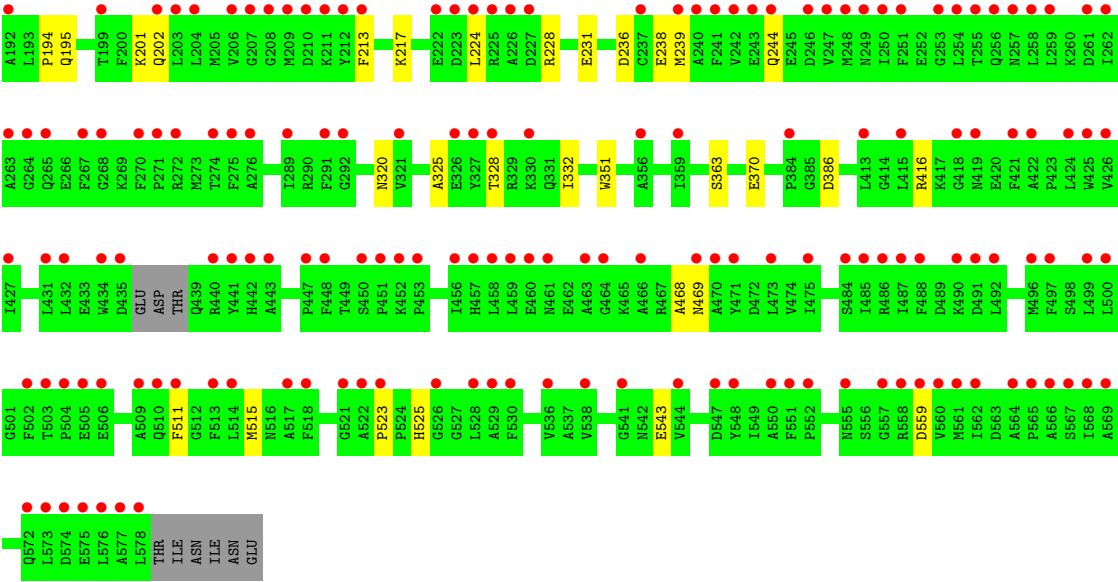


• Molecule 1: Aspartate-tRNA ligase



• Molecule 1: Aspartate-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.37Å 106.57Å 93.41Å 90.00° 100.91° 90.00°	Depositor
Resolution (Å)	36.07 – 2.15 36.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (36.07-2.15) 98.5 (36.07-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.18rc7 3834	Depositor
R, R_{free}	0.187 , 0.225 0.189 , 0.226	Depositor DCC
R_{free} test set	2019 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14257	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 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	0.39	0/4743	0.56	0/6407
1	B	0.36	0/4730	0.55	0/6395
1	C	0.26	0/4024	0.47	0/5479
All	All	0.35	0/13497	0.53	0/18281

There are no bond length outliers.

There are no bond angle outliers.

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	4635	0	4543	31	0
1	B	4622	0	4497	28	0
1	C	3941	0	3417	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	544	0	0	9	1
3	B	450	0	0	7	0
3	C	55	0	0	2	0
All	All	14257	0	12457	82	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 3.

All (82) 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:C:201:LYS:HD2	1:C:238:GLU:HB2	1.71	0.72
1:A:281:LYS:HE3	1:A:294[A]:GLU:HG2	1.70	0.71
1:B:445:HIS:ND1	3:B:807:HOH:O	2.26	0.69
1:B:441:TYR:OH	3:B:801:HOH:O	2.09	0.68
1:A:286:LYS:NZ	3:A:802:HOH:O	2.27	0.68
1:A:34:MET:HE3	1:A:51:ASP:HB2	1.78	0.66
1:A:462:GLU:HB3	1:A:465:LYS:HD2	1.79	0.64
1:C:181:VAL:HB	1:C:191:TYR:HB2	1.80	0.64
1:A:201:LYS:HD2	1:A:238:GLU:HB2	1.80	0.64
1:B:201:LYS:HD2	1:B:238:GLU:HB2	1.84	0.60
1:A:244:GLN:NE2	1:A:469:ASN:OD1	2.34	0.60
1:A:149[B]:GLN:OE1	3:A:801:HOH:O	2.17	0.60
1:B:528:LEU:HD21	1:B:530[B]:PHE:CE1	2.36	0.60
1:B:84:LYS:HG2	1:B:92:GLU:HA	1.83	0.59
1:C:468:ALA:O	3:C:601:HOH:O	2.18	0.56
1:B:99:LYS:NZ	3:B:811:HOH:O	2.37	0.56
1:B:481:GLY:HA3	1:B:530[B]:PHE:HD1	1.69	0.56
1:C:523:PRO:O	1:C:525:HIS:HD2	1.89	0.56
1:B:244:GLN:NE2	1:B:469:ASN:OD1	2.39	0.55
1:A:417:LYS:NZ	3:A:815:HOH:O	2.36	0.55
1:A:562:ILE:HD12	1:B:170:LYS:HB2	1.88	0.55
1:A:281:LYS:NZ	3:A:821:HOH:O	2.41	0.54
1:B:448:PHE:CZ	1:B:515[B]:MET:HE3	2.44	0.53
1:A:124:ARG:HH22	1:A:546:ARG:NH2	2.06	0.53
1:B:581:ASN:ND2	3:B:805:HOH:O	2.25	0.53
1:A:121:GLU:OE2	1:A:546:ARG:NH1	2.42	0.53
1:C:42:ARG:HG3	1:C:138:LYS:HD2	1.92	0.52
1:A:547:ASP:HB2	3:A:990:HOH:O	2.09	0.52
1:B:220:ARG:HB3	3:B:1092:HOH:O	2.09	0.51
1:C:180:VAL:HA	1:C:191:TYR:O	2.10	0.51
1:C:36:TRP:CD1	1:C:49:VAL:HG22	2.46	0.51
1:C:49:VAL:HG21	1:C:94:GLU:OE1	2.12	0.50
1:A:37:ILE:HD12	1:A:50:PHE:CE2	2.46	0.50
1:A:443:ALA:HB2	1:A:500:LEU:HD22	1.95	0.49
1:A:145:HIS:O	1:A:149[A]:GLN:HG2	2.13	0.48
1:B:124:ARG:HH12	1:B:546:ARG:HH22	1.61	0.48
1:C:224:LEU:HA	1:C:228:ARG:HB2	1.95	0.48
1:C:217:LYS:NZ	1:C:231:GLU:OE2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:O	1:A:194:PRO:HD3	2.14	0.48
1:A:575:GLU:CD	1:B:177:ARG:HE	2.22	0.47
1:B:171:SER:HB2	1:B:192:ALA:HB2	1.95	0.47
1:C:213:PHE:HA	1:C:236:ASP:O	2.14	0.47
1:A:519:LYS:HG3	1:B:107:GLU:HG3	1.97	0.46
1:A:353:LYS:NZ	3:A:814:HOH:O	2.35	0.46
1:B:453:PRO:HA	1:B:456:ILE:HD12	1.97	0.46
1:B:481:GLY:HA3	1:B:530[B]:PHE:CD1	2.50	0.46
1:C:328:THR:O	1:C:332:ILE:HG12	2.16	0.46
1:A:343:GLN:OE1	1:A:343:GLN:N	2.35	0.46
1:A:328:THR:O	1:A:332:ILE:HG12	2.16	0.45
1:B:167:VAL:O	1:B:194:PRO:HD3	2.15	0.45
1:B:515[B]:MET:HA	1:B:515[B]:MET:HE2	1.97	0.45
1:B:89:PRO:HD2	3:B:1107:HOH:O	2.15	0.45
1:C:40:ARG:HG3	1:C:45:ILE:HG12	1.99	0.45
1:C:511:PHE:O	1:C:515:MET:HG2	2.17	0.45
1:A:124:ARG:HD2	1:A:131:ASP:OD1	2.16	0.45
1:A:248:MET:HE3	1:A:425:TRP:CG	2.52	0.44
1:B:154:TYR:OH	3:B:802:HOH:O	2.20	0.44
1:B:174:GLU:H	1:B:174:GLU:CD	2.25	0.44
1:B:480:ILE:HG22	1:B:530[A]:PHE:HD1	1.83	0.44
1:C:244:GLN:HE22	1:C:469:ASN:HA	1.83	0.44
1:C:167:VAL:O	1:C:194:PRO:HD3	2.17	0.44
1:A:320:ASN:OD1	1:A:386:ASP:HB3	2.18	0.43
1:C:320:ASN:OD1	1:C:386:ASP:HB3	2.18	0.43
1:A:220:ARG:HB3	3:A:834:HOH:O	2.17	0.43
1:A:182:PRO:HD2	1:B:180:VAL:O	2.19	0.43
1:A:64:LYS:NZ	3:A:818:HOH:O	2.39	0.43
1:C:182:PRO:HA	1:C:189:GLN:O	2.18	0.43
1:C:160:PHE:HZ	1:C:239:MET:SD	2.42	0.43
1:C:559:ASP:HA	3:C:643:HOH:O	2.19	0.42
1:C:325:ALA:HB2	1:C:386:ASP:O	2.19	0.42
1:A:52:GLN:HB3	1:A:60:LEU:HG	2.02	0.42
1:B:523:PRO:O	1:B:525:HIS:HD2	2.02	0.42
1:B:117:THR:HG21	1:B:124:ARG:HD3	2.02	0.42
1:A:281:LYS:CE	1:A:294[A]:GLU:HG2	2.44	0.41
1:A:444:MET:HB3	3:A:1160:HOH:O	2.20	0.41
1:C:202:GLN:OE1	1:C:525:HIS:HE1	2.01	0.41
1:C:351:TRP:NE1	1:C:363:SER:HB3	2.35	0.41
1:C:40:ARG:HG2	1:C:41:ASP:N	2.35	0.41
1:C:176:ALA:HB3	1:C:195:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HD3	1:C:236:ASP:OD2	2.20	0.41
1:B:480:ILE:HG22	1:B:530[A]:PHE:CD1	2.57	0.40
1:C:416:ARG:NH2	1:C:543:GLU:OE2	2.42	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)
3:A:859:HOH:O	3:A:1193:HOH:O[1_554]	2.17	0.03

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	585/592 (99%)	569 (97%)	16 (3%)	0	100	100
1	B	585/592 (99%)	572 (98%)	13 (2%)	0	100	100
1	C	537/592 (91%)	524 (98%)	13 (2%)	0	100	100
All	All	1707/1776 (96%)	1665 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	489/509 (96%)	482 (99%)	7 (1%)	59	66
1	B	485/509 (95%)	481 (99%)	4 (1%)	73	79
1	C	343/509 (67%)	341 (99%)	2 (1%)	78	84
All	All	1317/1527 (86%)	1304 (99%)	13 (1%)	68	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	150	LYS
1	A	212	TYR
1	A	227	ASP
1	A	228	ARG
1	A	465	LYS
1	A	490	LYS
1	B	149	GLN
1	B	212	TYR
1	B	227	ASP
1	B	456	ILE
1	C	40	ARG
1	C	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	186	ASN
1	A	214	GLN
1	B	73	GLN
1	B	149	GLN
1	B	214	GLN
1	B	244	GLN
1	B	355	GLN
1	B	469	ASN
1	C	244	GLN
1	C	355	GLN
1	C	525	HIS

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 ⓘ

2 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	SO4	A	700	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	B	700	-	4,4,4	0.26	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	583/592 (98%)	-0.27	10 (1%) 69 73	19, 36, 55, 109	4 (0%)
1	B	583/592 (98%)	-0.13	10 (1%) 69 73	20, 40, 68, 133	4 (0%)
1	C	549/592 (92%)	2.00	276 (50%) 0 1	40, 88, 139, 219	0
All	All	1715/1776 (96%)	0.50	296 (17%) 4 4	19, 45, 118, 219	8 (0%)

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	TYR	7.3
1	C	560	VAL	5.9
1	C	190	PHE	5.8
1	C	207	GLY	5.7
1	C	578	LEU	5.6
1	C	45	ILE	5.6
1	C	576	LEU	5.5
1	C	59	LEU	5.5
1	C	39	LEU	5.3
1	C	93	ILE	5.2
1	C	161	ILE	5.2
1	C	97	VAL	5.2
1	C	241	PHE	5.0
1	C	48	LEU	4.9
1	C	136	PRO	4.8
1	C	2	PHE	4.8
1	C	154	TYR	4.8
1	C	96	LEU	4.7
1	C	182	PRO	4.7
1	C	464	GLY	4.7
1	C	255	THR	4.7
1	C	425	TRP	4.7
1	C	435	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	31	LYS	4.6
1	C	36	TRP	4.5
1	C	250	ILE	4.5
1	C	450	SER	4.4
1	C	9	GLU	4.4
1	C	421	PHE	4.4
1	C	242	VAL	4.4
1	C	10	LEU	4.4
1	C	130	LEU	4.3
1	C	577	ALA	4.3
1	C	562	ILE	4.3
1	C	180	VAL	4.2
1	C	191	TYR	4.2
1	B	0	HIS	4.2
1	C	24	TRP	4.2
1	C	565	PRO	4.2
1	C	50	PHE	4.2
1	C	566	ALA	4.1
1	C	499	LEU	4.1
1	C	160	PHE	4.1
1	C	247	VAL	4.1
1	C	174	GLU	4.1
1	C	557	GLY	4.0
1	C	564	ALA	4.0
1	C	572	GLN	4.0
1	C	206	VAL	4.0
1	C	60	LEU	4.0
1	C	463	ALA	3.9
1	C	43	TYR	3.9
1	C	95	ILE	3.9
1	C	427	ILE	3.9
1	C	530	PHE	3.8
1	C	568	ILE	3.8
1	C	134	ARG	3.8
1	C	327	TYR	3.8
1	A	0	HIS	3.8
1	C	125	MET	3.8
1	C	226	ALA	3.7
1	C	244	GLN	3.7
1	C	72	ILE	3.7
1	C	203	LEU	3.7
1	C	185	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	3.7
1	C	263	ALA	3.7
1	C	111	PHE	3.6
1	C	143	PHE	3.6
1	C	66	LEU	3.6
1	C	159	GLY	3.6
1	C	264	GLY	3.6
1	C	573	LEU	3.6
1	C	261	ASP	3.5
1	C	151	VAL	3.5
1	C	62	GLU	3.5
1	C	270	PHE	3.5
1	C	46	THR	3.5
1	C	419	ASN	3.5
1	A	582	ILE	3.5
1	C	147	ILE	3.4
1	C	267	PHE	3.4
1	C	441	TYR	3.4
1	C	6	THR	3.4
1	C	37	ILE	3.4
1	C	448	PHE	3.4
1	C	528	LEU	3.4
1	C	243	GLU	3.4
1	C	223	ASP	3.4
1	C	183	SER	3.4
1	C	35	ILE	3.4
1	C	187	PRO	3.3
1	C	569	ALA	3.3
1	C	249	ASN	3.3
1	C	555	ASN	3.3
1	C	451	PRO	3.3
1	C	78	VAL	3.2
1	C	63	ALA	3.2
1	C	155	LEU	3.2
1	C	213	PHE	3.2
1	C	518	PHE	3.2
1	C	184	ARG	3.2
1	C	486	ARG	3.2
1	C	113	ILE	3.2
1	C	262	ILE	3.2
1	C	222	GLU	3.2
1	C	186	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	3.2
1	C	559	ASP	3.2
1	C	132	ILE	3.1
1	C	491	ASP	3.1
1	C	237	CYS	3.1
1	C	137	VAL	3.1
1	C	253	GLY	3.1
1	C	415	LEU	3.0
1	C	424	LEU	3.0
1	C	469	ASN	3.0
1	C	64	LYS	3.0
1	C	74	VAL	3.0
1	C	272	ARG	3.0
1	C	102	ILE	3.0
1	C	109	PRO	3.0
1	C	251	PHE	3.0
1	B	226	ALA	3.0
1	C	443	ALA	3.0
1	C	413	LEU	3.0
1	C	538	VAL	3.0
1	C	418	GLY	3.0
1	C	487	ILE	3.0
1	C	126	LYS	3.0
1	C	61	GLU	2.9
1	C	240	ALA	2.9
1	C	517	ALA	2.9
1	C	1	MET	2.9
1	C	40	ARG	2.9
1	C	99	LYS	2.9
1	C	141	LEU	2.9
1	C	541	GLY	2.9
1	C	488	PHE	2.9
1	C	452	LYS	2.8
1	C	265	GLN	2.8
1	C	120	GLY	2.8
1	C	210	ASP	2.8
1	C	514	LEU	2.8
1	C	506	GLU	2.8
1	C	79	ILE	2.8
1	C	110	PRO	2.8
1	C	510	GLN	2.8
1	C	521	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	49	VAL	2.8
1	C	44	GLY	2.8
1	C	422	ALA	2.8
1	C	65	LYS	2.8
1	C	181	VAL	2.8
1	C	128	ARG	2.7
1	C	509	ALA	2.7
1	C	71	VAL	2.7
1	C	135	ASN	2.7
1	C	359	ILE	2.7
1	C	567	SER	2.7
1	C	30	ASP	2.7
1	C	58	ALA	2.7
1	C	117	THR	2.7
1	C	432	LEU	2.7
1	C	442	HIS	2.7
1	C	475	ILE	2.7
1	C	189	GLN	2.7
1	C	239	MET	2.7
1	C	248	MET	2.7
1	C	131	ASP	2.7
1	C	227	ASP	2.7
1	C	330	LYS	2.7
1	C	70	PHE	2.6
1	C	459	LEU	2.6
1	B	173	PRO	2.6
1	C	552	PRO	2.6
1	B	227	ASP	2.6
1	C	426	VAL	2.6
1	C	209	MET	2.6
1	C	259	LEU	2.6
1	C	447	PRO	2.6
1	C	29	ARG	2.6
1	C	225	ARG	2.6
1	C	67	GLY	2.6
1	C	108	LEU	2.6
1	C	211	LYS	2.6
1	C	453	PRO	2.6
1	C	246	ASP	2.6
1	C	551	PHE	2.6
1	C	456	ILE	2.6
1	C	208	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	461	ASN	2.6
1	C	484	SER	2.6
1	C	513	PHE	2.5
1	C	561	MET	2.5
1	C	440	ARG	2.5
1	C	558	ARG	2.5
1	C	106	SER	2.5
1	C	291	PHE	2.5
1	C	28	ILE	2.5
1	C	212	TYR	2.5
1	C	326	GLU	2.5
1	C	470	ALA	2.5
1	C	504	PRO	2.5
1	C	550	ALA	2.5
1	C	492	LEU	2.5
1	C	256	GLN	2.5
1	B	438	THR	2.5
1	C	276	ALA	2.5
1	C	103	LEU	2.5
1	C	458	LEU	2.5
1	C	268	GLY	2.5
1	C	485	ILE	2.5
1	A	227	ASP	2.4
1	C	471	TYR	2.4
1	C	224	LEU	2.4
1	C	503	THR	2.4
1	C	271	PRO	2.4
1	C	384	PRO	2.4
1	C	5	HIS	2.4
1	C	431	LEU	2.4
1	C	179	PHE	2.4
1	C	202	GLN	2.4
1	C	115	ASP	2.4
1	C	522	ALA	2.4
1	C	473	LEU	2.4
1	C	121	GLU	2.4
1	C	547	ASP	2.4
1	C	289	ILE	2.4
1	C	548	TYR	2.3
1	C	98	GLU	2.3
1	C	460	GLU	2.3
1	C	529	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	100	LEU	2.3
1	C	500	LEU	2.3
1	C	497	PHE	2.3
1	C	56	SER	2.3
1	C	172	THR	2.3
1	C	158	GLN	2.3
1	C	7	ASN	2.3
1	C	257	ASN	2.3
1	C	188	GLY	2.3
1	C	292	GLY	2.3
1	C	457	HIS	2.3
1	C	27	THR	2.3
1	C	466	ALA	2.3
1	A	264	GLY	2.3
1	B	223	ASP	2.3
1	B	1	MET	2.3
1	C	544	VAL	2.3
1	C	199	THR	2.3
1	C	526	GLY	2.3
1	C	258	LEU	2.3
1	C	4	THR	2.2
1	C	21	LEU	2.2
1	C	204	LEU	2.2
1	C	145	HIS	2.2
1	B	225	ARG	2.2
1	C	42	ARG	2.2
1	C	22	SER	2.2
1	C	3	ARG	2.2
1	A	33	PHE	2.2
1	C	92	GLU	2.2
1	C	176	ALA	2.2
1	C	192	ALA	2.2
1	C	523	PRO	2.1
1	B	582	ILE	2.1
1	C	575	GLU	2.1
1	A	185	MET	2.1
1	C	574	ASP	2.1
1	C	502	PHE	2.1
1	C	23	GLY	2.1
1	A	263	ALA	2.1
1	C	505	GLU	2.1
1	C	8	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	19	VAL	2.1
1	C	490	LYS	2.1
1	C	356	ALA	2.1
1	C	496	MET	2.1
1	C	146	LYS	2.1
1	C	275	PHE	2.1
1	C	536	VAL	2.1
1	B	342	PRO	2.0
1	C	142	ILE	2.0
1	C	321	VAL	2.0
1	C	511	PHE	2.0
1	C	171	SER	2.0
1	C	434	TRP	2.0
1	A	30	ASP	2.0
1	C	41	ASP	2.0
1	C	178	ASP	2.0
1	A	225	ARG	2.0
1	C	101	THR	2.0
1	C	173	PRO	2.0
1	C	274	THR	2.0
1	C	328	THR	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	700	5/5	0.74	0.19	84,85,86,87	5
2	SO4	A	700	5/5	0.94	0.08	51,53,54,56	5

6.5 Other polymers [i](#)

There are no such residues in this entry.