



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:59 pm BST

PDB ID : 6WOM
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

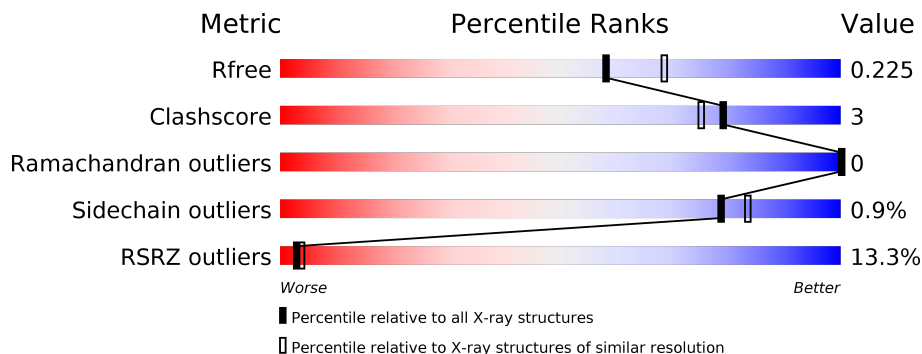
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 on 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% 91% 7%
1	B	592	 3% 93% 5%
1	C	592	 33% 85% 8% 7%

2 Entry composition i

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
			Total	C	N	O	S			
1	A	583	Total 4635	C 2957	N 785	O 873	S 20	0	4	0
1	B	583	Total 4622	C 2948	N 779	O 874	S 21	0	4	0
1	C	549	Total 3941	C 2499	N 680	O 744	S 18	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

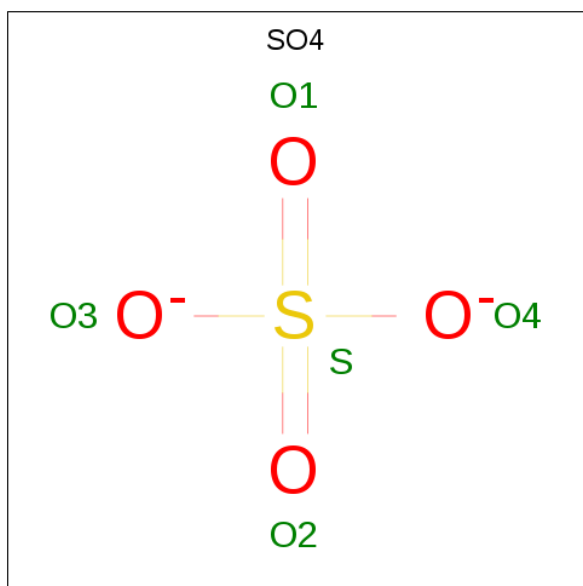
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A1T3DDI2
A	-6	ALA	-	expression tag	UNP A0A1T3DDI2
A	-5	HIS	-	expression tag	UNP A0A1T3DDI2
A	-4	HIS	-	expression tag	UNP A0A1T3DDI2
A	-3	HIS	-	expression tag	UNP A0A1T3DDI2
A	-2	HIS	-	expression tag	UNP A0A1T3DDI2
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 (three-letter code: SO4) (formula: O₄S).



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

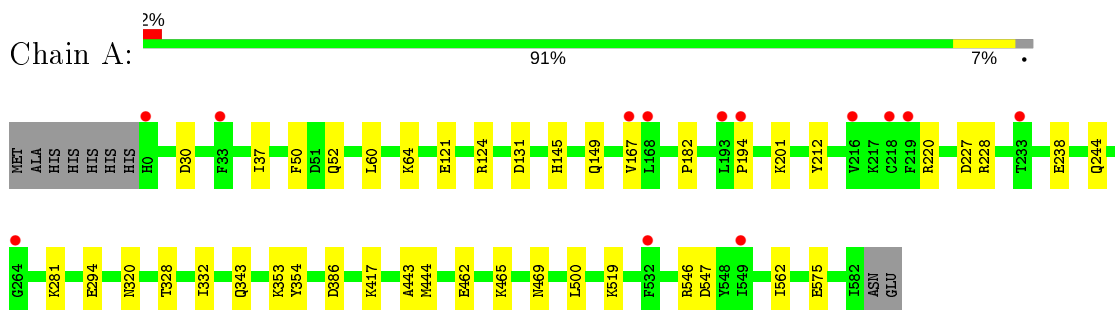
- Molecule 3 is water.

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

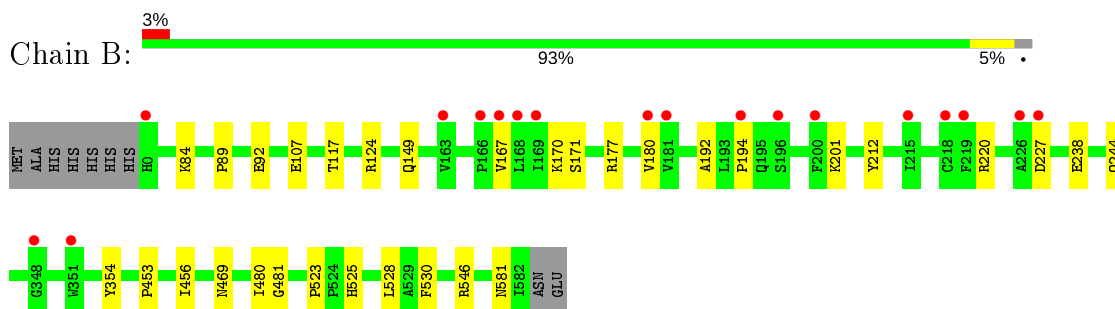
3 Residue-property plots [i](#)

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

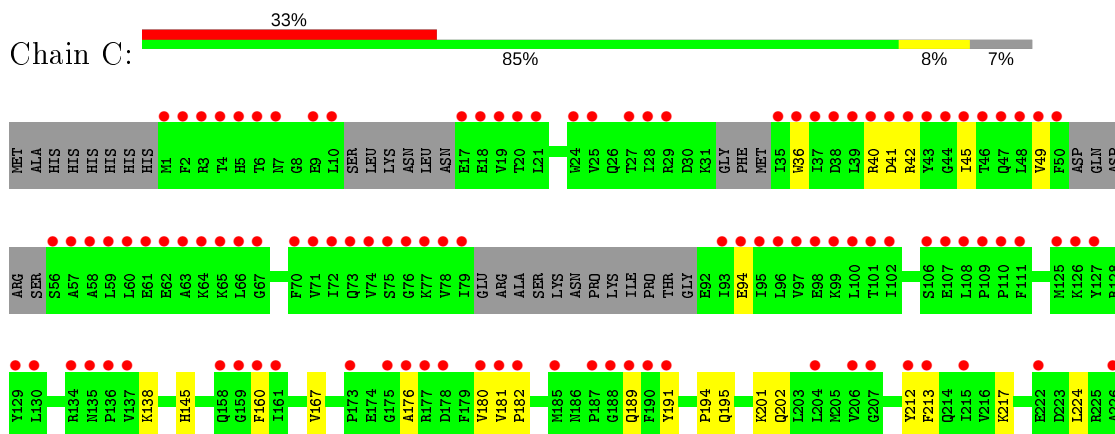
- Molecule 1: Aspartate-tRNA ligase

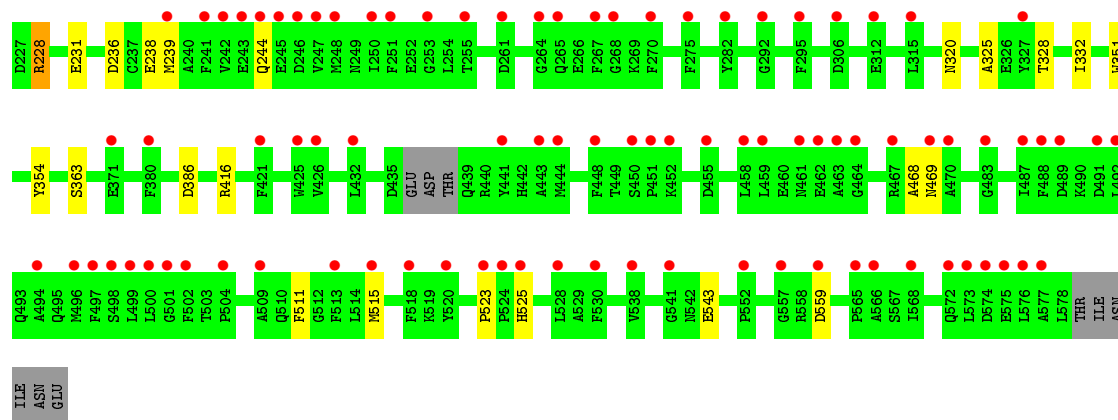


- Molecule 1: Aspartate-tRNA ligase



- 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 48.35 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (36.07-2.15) 98.5 (48.35-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.18rc7 3834	Depositor
R, R_{free}	0.187 , 0.225 0.187 , 0.225	Depositor DCC
R_{free} test set	2019 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.46	0/4743	0.60	0/6407
1	B	0.43	0/4730	0.59	0/6395
1	C	0.32	1/4024 (0.0%)	0.51	0/5479
All	All	0.41	1/13497 (0.0%)	0.57	0/18281

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	ARG	C-N	-5.16	1.22	1.34

There are no bond angle outliers.

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	4635	0	4543	28	0
1	B	4622	0	4497	21	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	8	1
3	B	450	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	55	0	0	2	0
All	All	14257	0	12457	72	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 (72) 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: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:A:417:LYS:NZ	3:A:815:HOH:O	2.36	0.59
1:B:84:LYS:HG2	1:B:92:GLU:HA	1.83	0.59
1:A:353:LYS:NZ	3:A:814:HOH:O	2.35	0.58
1:C:468:ALA:O	3:C:601:HOH:O	2.18	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:562:ILE:HD12	1:B:170:LYS:HB2	1.88	0.55
1:C:217:LYS:NZ	1:C:231:GLU:OE2	2.26	0.54
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:A:281:LYS:NZ	3:A:821:HOH:O	2.41	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:64:LYS:NZ	3:A:818:HOH:O	2.39	0.49
1:A:145:HIS:O	1:A:149[A]:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:167:VAL:O	1:A:194:PRO:HD3	2.14	0.48
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: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:N	1:A:343:GLN:OE1	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: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: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:C:182:PRO:HA	1:C:189:GLN:O	2.18	0.43
1:A:575:GLU:CD	1:B:177:ARG:HE	2.22	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
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 sym-

metry 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%)	484 (99%)	5 (1%)	76	81
1	B	485/509 (95%)	481 (99%)	4 (1%)	81	86
1	C	343/509 (67%)	340 (99%)	3 (1%)	78	83
All	All	1317/1527 (86%)	1305 (99%)	12 (1%)	78	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	212	TYR
1	A	227	ASP
1	A	228	ARG
1	A	354	TYR
1	B	149	GLN
1	B	212	TYR
1	B	227	ASP
1	B	354	TYR
1	C	145	HIS
1	C	212	TYR
1	C	354	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	GLN
1	B	469	ASN
1	C	7	ASN
1	C	244	GLN
1	C	525	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.14	0	6,6,6	0.16	0
2	SO4	B	700	-	4,4,4	0.16	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 [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	583/592 (98%)	0.13	13 (2%) 62 69	25, 36, 55, 109	0
1	B	583/592 (98%)	0.26	18 (3%) 49 58	25, 40, 68, 133	0
1	C	549/592 (92%)	1.74	197 (35%) 0 0	40, 88, 139, 219	0
All	All	1715/1776 (96%)	0.69	228 (13%) 3 4	25, 45, 118, 219	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	8.8
1	C	96	LEU	8.4
1	C	129	TYR	7.8
1	C	97	VAL	7.5
1	C	425	TRP	7.4
1	C	190	PHE	7.4
1	C	49	VAL	7.1
1	C	4	THR	6.6
1	C	76	GLY	6.6
1	C	46	THR	6.6
1	C	64	LYS	6.4
1	C	79	ILE	6.4
1	C	565	PRO	6.3
1	C	37	ILE	6.2
1	C	10	LEU	6.2
1	C	36	TRP	6.1
1	C	577	ALA	6.1
1	C	93	ILE	6.0
1	C	450	SER	5.9
1	C	59	LEU	5.8
1	C	463	ALA	5.7
1	C	2	PHE	5.7
1	C	58	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	65	LYS	5.5
1	C	50	PHE	5.3
1	C	78	VAL	5.2
1	C	5	HIS	5.1
1	C	99	LYS	5.1
1	C	95	ILE	4.9
1	C	21	LEU	4.9
1	C	130	LEU	4.9
1	C	499	LEU	4.6
1	C	74	VAL	4.6
1	C	100	LEU	4.6
1	C	28	ILE	4.5
1	C	18	GLU	4.5
1	C	19	VAL	4.5
1	C	45	ILE	4.4
1	C	101	THR	4.4
1	C	250	ILE	4.3
1	C	441	TYR	4.2
1	C	189	GLN	4.2
1	C	62	GLU	4.2
1	C	29	ARG	4.2
1	C	109	PRO	4.1
1	C	464	GLY	4.1
1	C	576	LEU	4.1
1	C	98	GLU	4.1
1	C	504	PRO	4.0
1	C	206	VAL	4.0
1	C	134	ARG	4.0
1	C	261	ASP	4.0
1	C	421	PHE	4.0
1	C	557	GLY	4.0
1	C	242	VAL	4.0
1	C	264	GLY	4.0
1	C	159	GLY	4.0
1	C	204	LEU	3.9
1	C	57	ALA	3.9
1	C	173	PRO	3.9
1	C	20	THR	3.9
1	C	136	PRO	3.8
1	C	182	PRO	3.8
1	C	61	GLU	3.8
1	C	111	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	39	LEU	3.7
1	C	6	THR	3.7
1	C	66	LEU	3.7
1	C	270	PHE	3.7
1	C	327	TYR	3.7
1	C	110	PRO	3.7
1	C	572	GLN	3.6
1	C	60	LEU	3.6
1	C	160	PHE	3.6
1	C	239	MET	3.6
1	C	180	VAL	3.6
1	C	538	VAL	3.5
1	C	267	PHE	3.5
1	C	187	PRO	3.4
1	C	67	GLY	3.4
1	C	176	ALA	3.4
1	C	568	ILE	3.4
1	C	207	GLY	3.4
1	B	226	ALA	3.4
1	C	108	LEU	3.3
1	C	498	SER	3.3
1	C	501	GLY	3.3
1	C	312	GLU	3.2
1	C	246	ASP	3.2
1	C	63	ALA	3.2
1	C	44	GLY	3.2
1	C	488	PHE	3.2
1	C	25	VAL	3.2
1	C	94	GLU	3.2
1	B	167	VAL	3.2
1	C	247	VAL	3.2
1	C	24	TRP	3.1
1	C	459	LEU	3.1
1	C	35	ILE	3.1
1	C	125	MET	3.1
1	C	17	GLU	3.1
1	C	491	ASP	3.1
1	C	432	LEU	3.1
1	C	47	GLN	3.1
1	C	9	GLU	3.1
1	C	226	ALA	3.0
1	C	541	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	492	LEU	3.0
1	C	27	THR	3.0
1	C	43	TYR	3.0
1	A	219	PHE	2.9
1	C	40	ARG	2.9
1	B	168	LEU	2.9
1	A	33	PHE	2.9
1	C	470	ALA	2.9
1	C	106	SER	2.9
1	A	167	VAL	2.9
1	C	241	PHE	2.9
1	C	559	ASP	2.8
1	A	193	LEU	2.8
1	C	42	ARG	2.8
1	C	253	GLY	2.8
1	C	255	THR	2.8
1	A	0	HIS	2.8
1	C	489	ASP	2.8
1	B	351	TRP	2.8
1	B	219	PHE	2.8
1	C	497	PHE	2.8
1	C	315	LEU	2.8
1	C	426	VAL	2.7
1	C	380	PHE	2.7
1	C	38	ASP	2.7
1	C	573	LEU	2.7
1	C	275	PHE	2.7
1	A	168	LEU	2.7
1	C	525	HIS	2.7
1	C	243	GLU	2.6
1	A	264	GLY	2.6
1	A	233	THR	2.6
1	C	513	PHE	2.6
1	B	348	GLY	2.6
1	C	245	GLU	2.6
1	C	70	PHE	2.6
1	C	72	ILE	2.6
1	C	461	ASN	2.5
1	B	218	CYS	2.5
1	C	71	VAL	2.5
1	C	574	ASP	2.5
1	C	520	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	502	PHE	2.5
1	C	451	PRO	2.5
1	C	56	SER	2.5
1	C	469	ASN	2.5
1	C	175	GLY	2.5
1	C	524	PRO	2.5
1	C	7	ASN	2.5
1	B	169	ILE	2.4
1	C	443	ALA	2.4
1	C	496	MET	2.4
1	C	500	LEU	2.4
1	C	244	GLN	2.4
1	C	222	GLU	2.4
1	C	494	ALA	2.4
1	C	566	ALA	2.4
1	C	452	LYS	2.4
1	C	552	PRO	2.4
1	C	191	TYR	2.4
1	C	181	VAL	2.4
1	C	515	MET	2.4
1	C	487	ILE	2.4
1	C	458	LEU	2.4
1	B	181	VAL	2.4
1	C	509	ALA	2.4
1	C	528	LEU	2.3
1	C	178	ASP	2.3
1	C	161	ILE	2.3
1	B	180	VAL	2.3
1	C	41	ASP	2.3
1	B	194	PRO	2.3
1	A	216	VAL	2.3
1	C	292	GLY	2.3
1	C	575	GLU	2.3
1	B	196	SER	2.3
1	C	126	LYS	2.3
1	B	166	PRO	2.3
1	C	73	GLN	2.3
1	C	137	VAL	2.3
1	A	194	PRO	2.3
1	C	444	MET	2.2
1	C	177	ARG	2.2
1	C	102	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	2.2
1	C	462	GLU	2.2
1	C	1	MET	2.2
1	C	135	ASN	2.2
1	A	532	PHE	2.2
1	C	295	PHE	2.2
1	C	215	ILE	2.2
1	C	483	GLY	2.2
1	C	467	ARG	2.2
1	C	455	ASP	2.2
1	A	549	ILE	2.1
1	C	107	GLU	2.1
1	C	212	TYR	2.1
1	C	77	LYS	2.1
1	B	0	HIS	2.1
1	C	127	TYR	2.1
1	C	188	GLY	2.1
1	C	268	GLY	2.1
1	C	75	SER	2.1
1	C	448	PHE	2.1
1	A	218	CYS	2.1
1	B	227	ASP	2.1
1	C	265	GLN	2.1
1	B	215	ILE	2.1
1	C	185	MET	2.1
1	C	530	PHE	2.1
1	C	282	TYR	2.1
1	C	371	GLU	2.1
1	B	200	PHE	2.1
1	C	518	PHE	2.1
1	C	306	ASP	2.0
1	C	251	PHE	2.0
1	C	3	ARG	2.0
1	C	158	GLN	2.0
1	C	248	MET	2.0
1	C	523	PRO	2.0
1	C	213	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	SO4	B	700	5/5	0.80	0.31	84,85,86,87	5
2	SO4	A	700	5/5	0.97	0.20	51,53,54,56	5

6.5 Other polymers [i](#)

There are no such residues in this entry.