



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2017 – 08:45 PM EDT

PDB ID : 5K4H
Title : Wolinella succinogenes L-asparaginase S121 + L-Glutamic acid
Authors : Nguyen, H.A.; Lave, A.
Deposited on : 2016-05-20
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

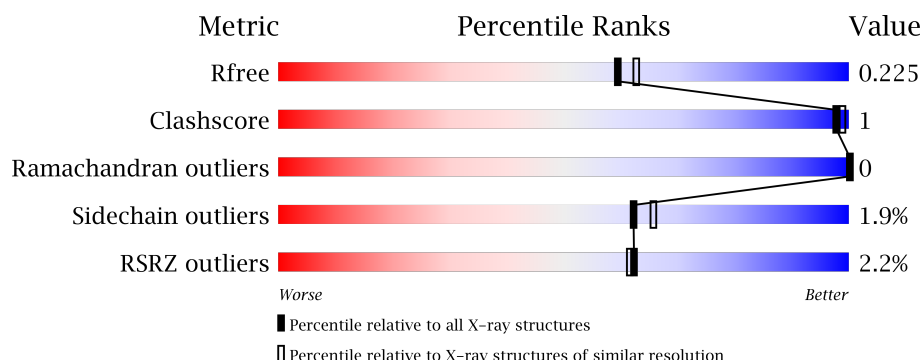
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



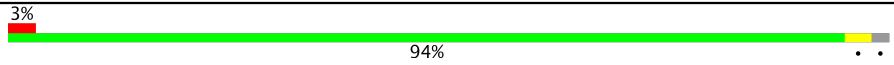
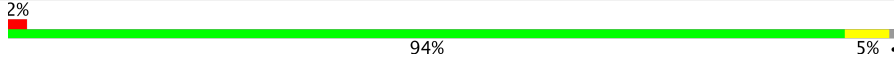
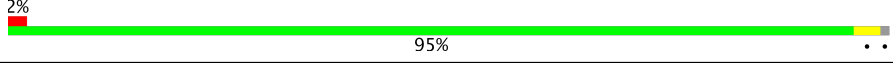
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	330	<div> <div>0.1%</div> <div>95%</div> </div>
1	B	330	<div> <div>3%</div> <div>93%</div> </div>
1	C	330	<div> <div>4%</div> <div>92%</div> </div>
1	D	330	<div> <div>0.1%</div> <div>93%</div> </div>
1	E	330	<div> <div>2%</div> <div>93%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	330	
1	G	330	
1	H	330	

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
2	GLU	F	400	-	-	-	X
2	GLU	H	400	-	-	-	X

2 Entry composition

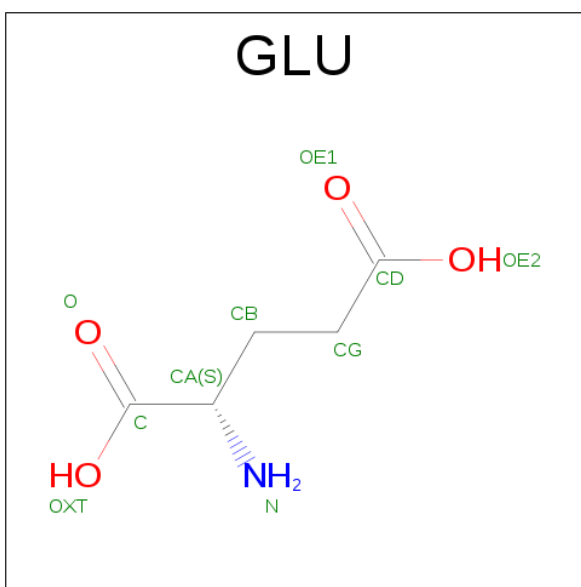
There are 3 unique types of molecules in this entry. The entry contains 20855 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2433	1524	418	483	8			
1	B	320	Total	C	N	O	S	0	0	0
			2380	1494	409	469	8			
1	C	316	Total	C	N	O	S	0	6	0
			2387	1498	411	470	8			
1	D	319	Total	C	N	O	S	0	0	0
			2368	1485	408	467	8			
1	E	321	Total	C	N	O	S	0	0	0
			2386	1497	410	471	8			
1	F	322	Total	C	N	O	S	0	0	0
			2393	1501	411	473	8			
1	G	328	Total	C	N	O	S	0	0	0
			2433	1524	418	483	8			
1	H	326	Total	C	N	O	S	0	0	0
			2418	1515	415	480	8			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	1
			20	10	2	8		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total	O	0	0
			217	217		
3	B	166	Total	O	0	0
			166	166		
3	C	184	Total	O	0	0
			184	184		
3	D	231	Total	O	0	0
			231	231		

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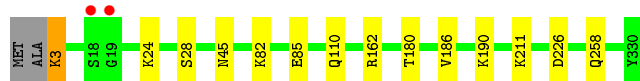
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	187	Total 187	O 187	0	0
3	F	187	Total 187	O 187	0	0
3	G	169	Total 169	O 169	0	0
3	H	226	Total 226	O 226	0	0

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.

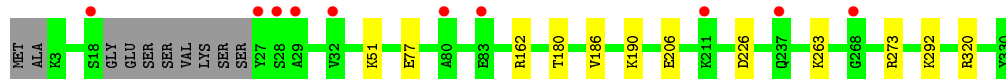
- Molecule 1: L-asparaginase

Chain A: 

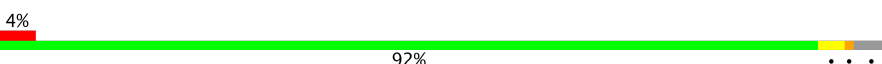


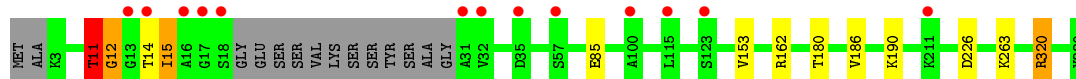
- Molecule 1: L-asparaginase

Chain B: 



- Molecule 1: L-asparaginase

Chain C: 



- Molecule 1: L-asparaginase

Chain D: 

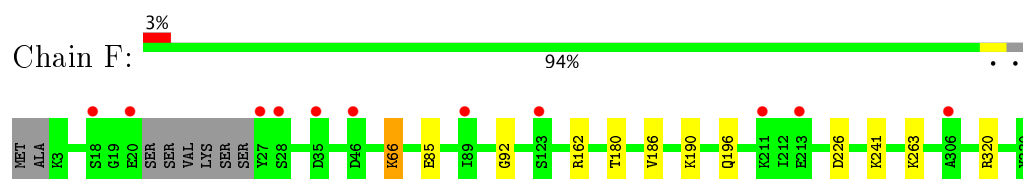


- Molecule 1: L-asparaginase

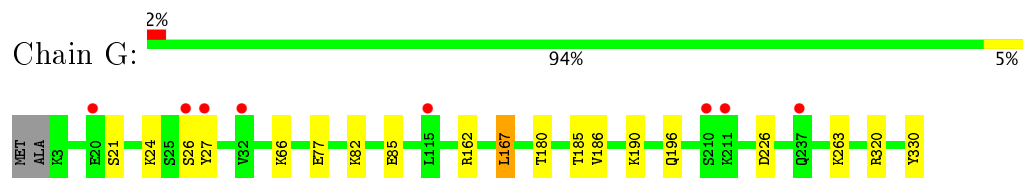
Chain E: 



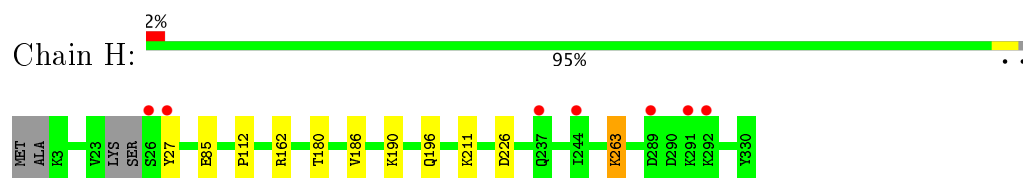
- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.54Å 84.18Å 120.55Å 87.22° 77.76° 70.84°	Depositor
Resolution (Å)	30.00 – 2.00 29.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.00) 93.9 (29.60-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.220 0.188 , 0.225	Depositor DCC
R_{free} test set	7436 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20855	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

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	0.65	0/2465	0.79	4/3340 (0.1%)
1	B	0.61	0/2411	0.80	7/3267 (0.2%)
1	C	0.67	2/2417 (0.1%)	0.85	11/3276 (0.3%)
1	D	0.69	2/2398 (0.1%)	0.81	6/3249 (0.2%)
1	E	0.65	0/2417	0.79	3/3275 (0.1%)
1	F	0.65	0/2424	0.77	3/3284 (0.1%)
1	G	0.63	0/2465	0.81	7/3340 (0.2%)
1	H	0.64	0/2449	0.77	2/3318 (0.1%)
All	All	0.65	4/19446 (0.0%)	0.80	43/26349 (0.2%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	GLU	CD-OE2	-8.07	1.16	1.25
1	D	262	GLU	CD-OE1	6.54	1.32	1.25
1	C	12[A]	GLY	CA-C	5.11	1.60	1.51
1	C	12[B]	GLY	CA-C	5.11	1.60	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	GLU	CG-CD-OE1	8.35	134.99	118.30
1	D	262	GLU	CG-CD-OE2	-7.81	102.68	118.30
1	A	3	LYS	CD-CE-NZ	7.57	129.10	111.70
1	D	167	LEU	CA-CB-CG	7.43	132.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	167	LEU	CA-CB-CG	7.29	132.07	115.30
1	C	162	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	B	77	GLU	CB-CA-C	7.12	124.63	110.40
1	G	77	GLU	CB-CA-C	7.08	124.56	110.40
1	E	167	LEU	CA-CB-CG	6.95	131.28	115.30
1	E	162	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	D	162	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	G	330	TYR	CA-C-O	-6.38	106.69	120.10
1	B	162	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	15[A]	ILE	N-CA-C	6.35	128.13	111.00
1	C	15[B]	ILE	N-CA-C	6.35	128.13	111.00
1	A	162	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	320	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	G	320	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	H	162	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	H	263	LYS	CG-CD-CE	6.07	130.10	111.90
1	C	15[A]	ILE	CA-CB-CG1	6.03	122.46	111.00
1	C	15[B]	ILE	CA-CB-CG1	6.03	122.46	111.00
1	E	320	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	3	LYS	CG-CD-CE	5.83	129.40	111.90
1	C	320	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	F	66	LYS	N-CA-CB	5.77	120.99	110.60
1	G	162	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	320	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	G	66	LYS	CA-CB-CG	5.54	125.60	113.40
1	C	162	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	11[A]	THR	CA-C-N	5.35	126.89	116.20
1	C	11[B]	THR	CA-C-N	5.35	126.89	116.20
1	F	162	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	162	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	15[A]	ILE	CA-C-N	5.32	128.90	117.20
1	C	15[B]	ILE	CA-C-N	5.32	128.90	117.20
1	G	320	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	292	LYS	CB-CG-CD	5.24	125.23	111.60
1	B	206	GLU	CG-CD-OE1	5.12	128.54	118.30
1	D	287	GLU	CG-CD-OE2	5.12	128.53	118.30
1	B	273	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	206	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	162	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11[B]	THR	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	2433	0	2488	6	0
1	B	2380	0	2436	3	0
1	C	2387	0	2446	10	0
1	D	2368	0	2427	3	0
1	E	2386	0	2441	5	0
1	F	2393	0	2445	4	0
1	G	2433	0	2488	5	0
1	H	2418	0	2469	6	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	20	0	10	1	0
2	D	10	0	5	0	0
2	E	10	0	5	0	0
2	F	10	0	5	1	0
2	G	10	0	5	0	0
2	H	10	0	5	0	0
3	A	217	0	0	2	0
3	B	166	0	0	1	0
3	C	184	0	0	5	0
3	D	231	0	0	1	0
3	E	187	0	0	1	0
3	F	187	0	0	0	0
3	G	169	0	0	1	0
3	H	226	0	0	1	0
All	All	20855	0	19685	35	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 1.

All (35) 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:12[A]:GLY:CA	3:C:503:HOH:O	2.19	0.89
1:C:12[A]:GLY:HA3	3:C:503:HOH:O	1.83	0.74
1:B:51:LYS:HE2	3:B:503:HOH:O	1.90	0.71
1:H:27:TYR:O	1:H:27:TYR:CD2	2.46	0.69
1:G:26:SER:O	1:G:27:TYR:C	2.31	0.68
1:C:320:ARG:NH1	3:C:502:HOH:O	2.31	0.62
1:C:153:VAL:HG12	3:C:618:HOH:O	2.01	0.61
1:A:110:GLN:HG2	3:A:503:HOH:O	1.99	0.61
1:C:14[A]:THR:N	2:C:400[A]:GLU:OE2	2.34	0.56
1:E:180:THR:O	1:G:180:THR:O	2.24	0.56
1:F:180:THR:O	1:H:180:THR:O	2.26	0.54
1:A:180:THR:O	1:C:180:THR:O	2.28	0.51
1:H:27:TYR:O	1:H:27:TYR:CG	2.63	0.50
1:C:11[A]:THR:H	1:C:12[A]:GLY:HA2	1.76	0.49
1:C:14[A]:THR:OG1	3:C:501:HOH:O	2.19	0.49
1:F:92:GLY:HA2	2:F:400:GLU:OE1	2.14	0.47
1:E:196:GLN:HE21	1:G:196:GLN:HE21	1.61	0.47
1:D:320:ARG:NH1	3:D:506:HOH:O	2.46	0.47
1:B:180:THR:O	1:D:180:THR:O	2.33	0.46
1:E:241:LYS:CE	3:E:683:HOH:O	2.63	0.46
1:A:258:GLN:NE2	3:A:501:HOH:O	2.28	0.45
1:C:11[A]:THR:N	1:C:12[A]:GLY:HA2	2.32	0.45
1:H:112:PRO:HA	3:H:511:HOH:O	2.17	0.44
1:E:186:VAL:HA	1:E:190:LYS:O	2.18	0.44
1:C:186:VAL:HA	1:C:190:LYS:O	2.18	0.43
1:A:186:VAL:HA	1:A:190:LYS:O	2.19	0.43
1:B:186:VAL:HA	1:B:190:LYS:O	2.19	0.42
1:F:186:VAL:HA	1:F:190:LYS:O	2.19	0.42
1:A:3:LYS:HE2	1:A:45:ASN:O	2.20	0.42
1:H:186:VAL:HA	1:H:190:LYS:O	2.20	0.42
1:D:186:VAL:HA	1:D:190:LYS:O	2.20	0.41
1:A:28:SER:O	1:E:123:SER:HB2	2.20	0.41
1:G:185:THR:HG22	3:G:548:HOH:O	2.21	0.41
1:G:186:VAL:HA	1:G:190:LYS:O	2.21	0.40
1:F:196:GLN:HE21	1:H:196:GLN:HE21	1.69	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	326/330 (99%)	315 (97%)	11 (3%)	0	100	100
1	B	316/330 (96%)	307 (97%)	9 (3%)	0	100	100
1	C	318/330 (96%)	305 (96%)	13 (4%)	0	100	100
1	D	315/330 (96%)	306 (97%)	9 (3%)	0	100	100
1	E	317/330 (96%)	305 (96%)	12 (4%)	0	100	100
1	F	318/330 (96%)	309 (97%)	9 (3%)	0	100	100
1	G	326/330 (99%)	313 (96%)	13 (4%)	0	100	100
1	H	322/330 (98%)	312 (97%)	10 (3%)	0	100	100
All	All	2558/2640 (97%)	2472 (97%)	86 (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	264/265 (100%)	259 (98%)	5 (2%)	62	66
1	B	257/265 (97%)	255 (99%)	2 (1%)	85	88
1	C	257/265 (97%)	252 (98%)	5 (2%)	62	66
1	D	256/265 (97%)	252 (98%)	4 (2%)	68	72
1	E	258/265 (97%)	253 (98%)	5 (2%)	62	66
1	F	258/265 (97%)	253 (98%)	5 (2%)	62	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	264/265 (100%)	257 (97%)	7 (3%)	50	51
1	H	262/265 (99%)	258 (98%)	4 (2%)	70	74
All	All	2076/2120 (98%)	2039 (98%)	37 (2%)	62	68

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	82	LYS
1	A	85	GLU
1	A	211	LYS
1	A	226	ASP
1	B	226	ASP
1	B	263	LYS
1	C	15[A]	ILE
1	C	15[B]	ILE
1	C	85	GLU
1	C	226	ASP
1	C	263	LYS
1	D	85	GLU
1	D	167	LEU
1	D	226	ASP
1	D	263	LYS
1	E	61	GLN
1	E	85	GLU
1	E	167	LEU
1	E	226	ASP
1	E	263	LYS
1	F	66	LYS
1	F	85	GLU
1	F	226	ASP
1	F	241	LYS
1	F	263	LYS
1	G	21	SER
1	G	24	LYS
1	G	82	LYS
1	G	85	GLU
1	G	167	LEU
1	G	226	ASP
1	G	263	LYS
1	H	85	GLU

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Mol	Chain	Res	Type
1	H	211	LYS
1	H	226	ASP
1	H	263	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	196	GLN
1	B	45	ASN
1	B	196	GLN
1	E	61	GLN
1	F	196	GLN
1	G	196	GLN

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](#)

9 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	GLU	A	400	-	1,9,9	0.09	0	1,11,11	2.53	1 (100%)
2	GLU	B	400	-	1,9,9	0.35	0	1,11,11	0.57	0
2	GLU	C	400[A]	-	1,9,9	0.29	0	1,11,11	0.01	0
2	GLU	C	400[B]	-	1,9,9	0.36	0	1,11,11	0.34	0
2	GLU	D	400	-	1,9,9	0.13	0	1,11,11	2.26	1 (100%)
2	GLU	E	400	-	1,9,9	0.08	0	1,11,11	1.79	0
2	GLU	F	400	-	1,9,9	0.27	0	1,11,11	0.24	0
2	GLU	G	400	-	1,9,9	0.18	0	1,11,11	2.30	1 (100%)
2	GLU	H	400	-	1,9,9	0.47	0	1,11,11	2.68	1 (100%)

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	GLU	A	400	-	-	0/3/9/9	0/0/0/0
2	GLU	B	400	-	-	0/3/9/9	0/0/0/0
2	GLU	C	400[A]	-	-	0/3/9/9	0/0/0/0
2	GLU	C	400[B]	-	-	0/3/9/9	0/0/0/0
2	GLU	D	400	-	-	0/3/9/9	0/0/0/0
2	GLU	E	400	-	-	0/3/9/9	0/0/0/0
2	GLU	F	400	-	-	0/3/9/9	0/0/0/0
2	GLU	G	400	-	-	0/3/9/9	0/0/0/0
2	GLU	H	400	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	GLU	CG-CB-CA	2.26	119.11	113.84
2	G	400	GLU	CG-CB-CA	2.30	119.20	113.84
2	A	400	GLU	CG-CB-CA	2.53	119.74	113.84
2	H	400	GLU	CG-CB-CA	2.68	120.09	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400[A]	GLU	1	0
2	F	400	GLU	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	328/330 (99%)	-0.17	2 (0%) 89 88	20, 33, 54, 70	0
1	B	320/330 (96%)	0.11	10 (3%) 49 49	23, 39, 63, 130	0
1	C	316/330 (95%)	-0.05	13 (4%) 38 38	21, 33, 60, 119	0
1	D	319/330 (96%)	-0.26	2 (0%) 89 88	19, 31, 49, 66	2 (0%)
1	E	321/330 (97%)	-0.18	5 (1%) 72 71	20, 32, 53, 72	3 (0%)
1	F	322/330 (97%)	-0.04	11 (3%) 46 46	21, 35, 54, 74	4 (1%)
1	G	328/330 (99%)	0.05	8 (2%) 59 59	21, 39, 59, 70	10 (3%)
1	H	326/330 (98%)	-0.18	7 (2%) 64 63	18, 32, 53, 86	1 (0%)
All	All	2580/2640 (97%)	-0.09	58 (2%) 62 61	18, 34, 57, 130	20 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	TYR	10.3
1	F	27	TYR	8.1
1	H	27	TYR	6.5
1	G	27	TYR	6.2
1	C	32	VAL	5.9
1	C	57	SER	5.4
1	H	26	SER	5.4
1	C	31	ALA	5.0
1	B	29	ALA	4.4
1	C	18	SER	4.2
1	B	28	SER	4.0
1	C	17	GLY	3.9
1	G	26	SER	3.7
1	C	16[A]	ALA	3.7
1	E	26	SER	3.6
1	B	237	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLY	3.3
1	B	32	VAL	3.2
1	B	18	SER	2.9
1	F	46	ASP	2.9
1	H	237	GLN	2.8
1	D	244	ILE	2.7
1	C	211	LYS	2.6
1	F	20	GLU	2.6
1	H	291	LYS	2.6
1	G	115	LEU	2.6
1	C	13[A]	GLY	2.6
1	B	83	GLU	2.5
1	H	289	ASP	2.4
1	F	89	ILE	2.4
1	F	18	SER	2.4
1	A	18	SER	2.4
1	F	306	ALA	2.4
1	F	211	LYS	2.4
1	G	20	GLU	2.4
1	G	237	GLN	2.3
1	G	211	LYS	2.3
1	C	35	ASP	2.3
1	C	115	LEU	2.3
1	C	123	SER	2.3
1	D	292	LYS	2.2
1	E	308	VAL	2.2
1	H	244	ILE	2.2
1	C	14[A]	THR	2.2
1	B	268	GLY	2.2
1	B	211	LYS	2.2
1	G	32	VAL	2.2
1	F	123	SER	2.2
1	F	213	GLU	2.1
1	F	35	ASP	2.1
1	F	28	SER	2.1
1	G	210	SER	2.1
1	H	292	LYS	2.1
1	B	80	ALA	2.1
1	E	211	LYS	2.1
1	E	27	TYR	2.0
1	E	309	LEU	2.0
1	C	100	ALA	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLU	F	400	10/10	0.91	0.12	2.48	39,46,64,69	0
2	GLU	H	400	10/10	0.95	0.13	2.33	27,46,54,60	0
2	GLU	C	400[B]	10/10	0.94	0.17	0.98	50,53,53,54	10
2	GLU	B	400	10/10	0.93	0.13	0.95	40,56,61,62	0
2	GLU	E	400	10/10	0.95	0.11	0.88	30,44,59,63	0
2	GLU	C	400[A]	10/10	0.94	0.17	0.58	29,34,42,49	10
2	GLU	D	400	10/10	0.97	0.09	-0.12	26,40,54,58	0
2	GLU	G	400	10/10	0.95	0.10	-0.61	42,46,56,61	0
2	GLU	A	400	10/10	0.97	0.09	-0.64	31,41,52,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.