



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:53 PM GMT

PDB ID : 4G3H
Title : Crystal structure of helicobacter pylori arginase
Authors : Zhang, J.; Zhang, X.; Li, D.; Hu, Y.; Zou, Q.; Wang, D.
Deposited on : 2012-07-13
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

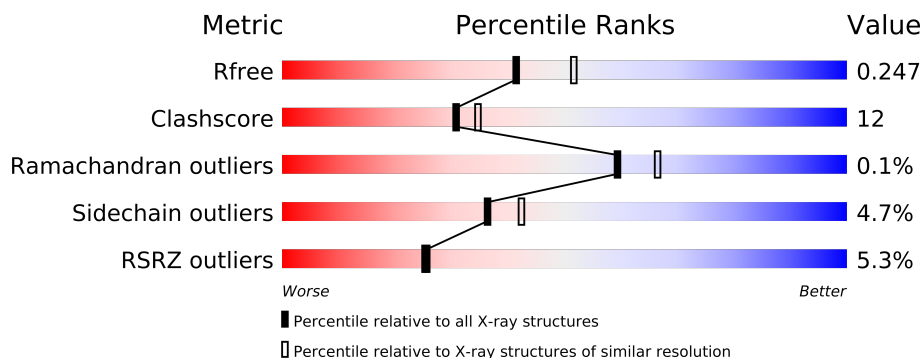
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	330	
1	B	330	
1	C	330	
1	D	330	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MN	B	501	-	X
2	MN	C	501	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10439 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Arginase (RocF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2419	1539	411	454	15			
1	B	305	Total	C	N	O	S	0	0	0
			2447	1551	417	465	14			
1	C	310	Total	C	N	O	S	6	0	0
			2491	1581	424	471	15			
1	D	300	Total	C	N	O	S	0	0	0
			2399	1524	407	453	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	EXPRESSION TAG	UNP O25949
A	324	GLU	-	EXPRESSION TAG	UNP O25949
A	325	HIS	-	EXPRESSION TAG	UNP O25949
A	326	HIS	-	EXPRESSION TAG	UNP O25949
A	327	HIS	-	EXPRESSION TAG	UNP O25949
A	328	HIS	-	EXPRESSION TAG	UNP O25949
A	329	HIS	-	EXPRESSION TAG	UNP O25949
A	330	HIS	-	EXPRESSION TAG	UNP O25949
B	323	LEU	-	EXPRESSION TAG	UNP O25949
B	324	GLU	-	EXPRESSION TAG	UNP O25949
B	325	HIS	-	EXPRESSION TAG	UNP O25949
B	326	HIS	-	EXPRESSION TAG	UNP O25949
B	327	HIS	-	EXPRESSION TAG	UNP O25949
B	328	HIS	-	EXPRESSION TAG	UNP O25949
B	329	HIS	-	EXPRESSION TAG	UNP O25949
B	330	HIS	-	EXPRESSION TAG	UNP O25949
C	323	LEU	-	EXPRESSION TAG	UNP O25949
C	324	GLU	-	EXPRESSION TAG	UNP O25949
C	325	HIS	-	EXPRESSION TAG	UNP O25949
C	326	HIS	-	EXPRESSION TAG	UNP O25949
C	327	HIS	-	EXPRESSION TAG	UNP O25949

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Chain	Residue	Modelled	Actual	Comment	Reference
C	328	HIS	-	EXPRESSION TAG	UNP O25949
C	329	HIS	-	EXPRESSION TAG	UNP O25949
C	330	HIS	-	EXPRESSION TAG	UNP O25949
D	323	LEU	-	EXPRESSION TAG	UNP O25949
D	324	GLU	-	EXPRESSION TAG	UNP O25949
D	325	HIS	-	EXPRESSION TAG	UNP O25949
D	326	HIS	-	EXPRESSION TAG	UNP O25949
D	327	HIS	-	EXPRESSION TAG	UNP O25949
D	328	HIS	-	EXPRESSION TAG	UNP O25949
D	329	HIS	-	EXPRESSION TAG	UNP O25949
D	330	HIS	-	EXPRESSION TAG	UNP O25949

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

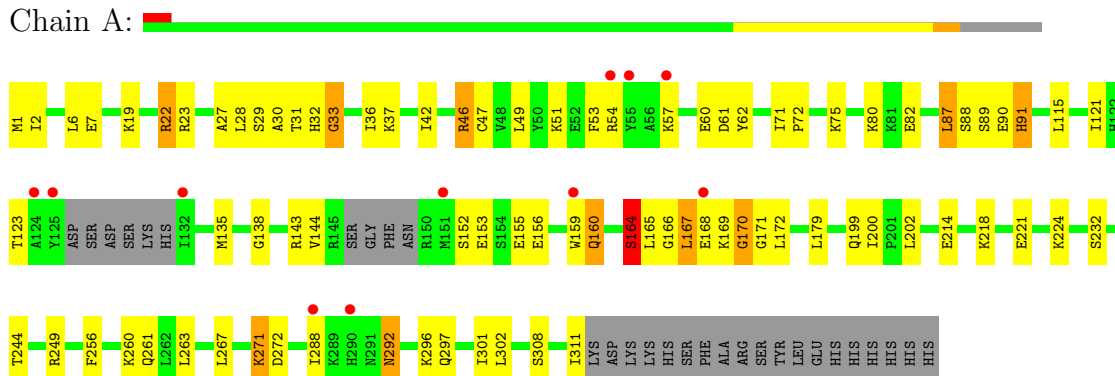
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	153	Total 153	O 153	0	0
3	C	168	Total 168	O 168	0	0
3	D	180	Total 180	O 180	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

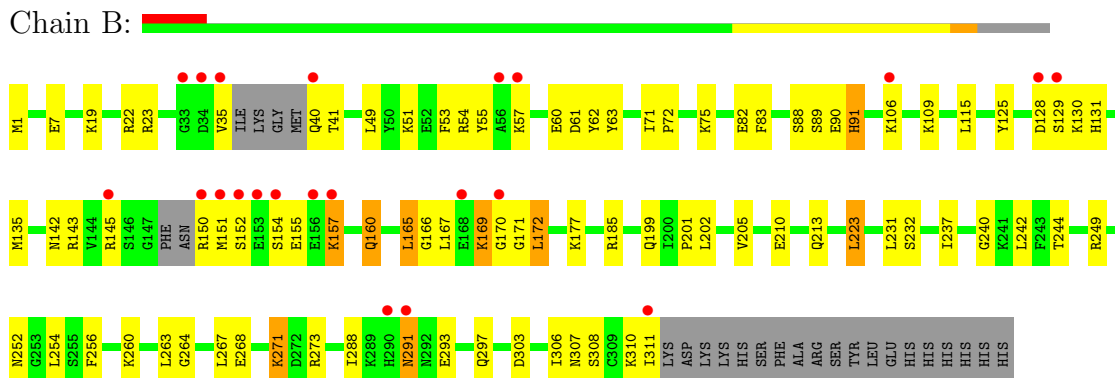
• Molecule 1: Arginase (RocF)

Chain A:



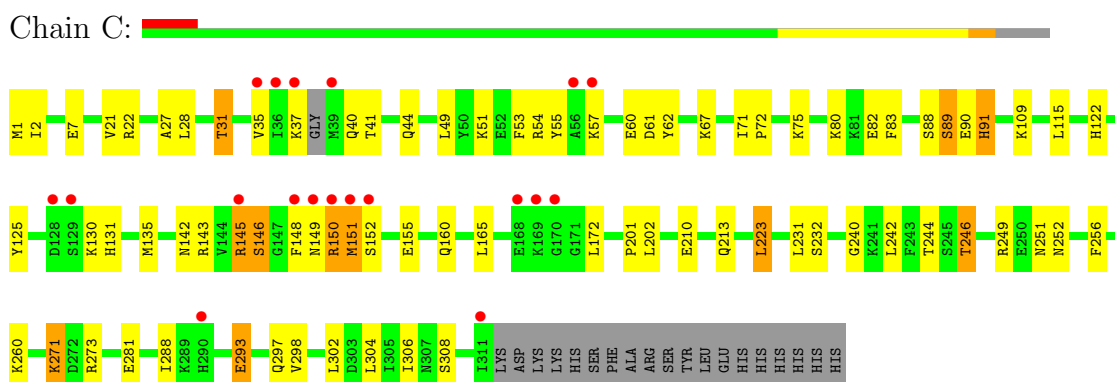
• Molecule 1: Arginase (RocF)

Chain B:

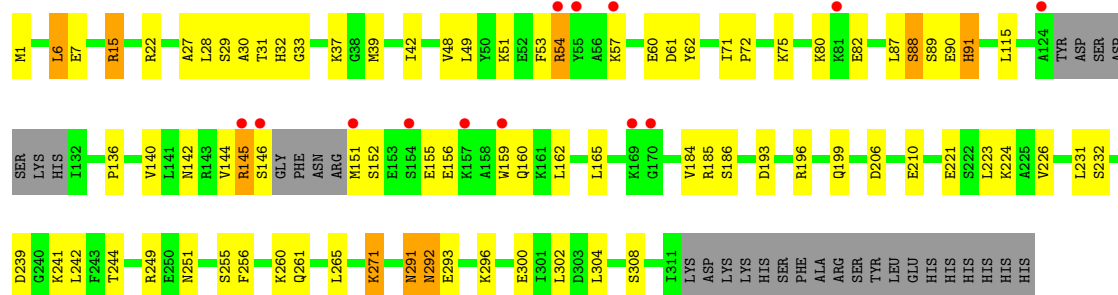


• Molecule 1: Arginase (RocF)

Chain C:



Chain D:



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.69Å 102.24Å 148.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.20 34.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.90-2.20) 99.9 (34.92-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.230 0.208 , 0.247	Depositor DCC
R_{free} test set	7448 reflections (10.10%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	1.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	7 of 73768 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.93 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5344e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.22	35/2453 (1.4%)	0.78	10/3289 (0.3%)
1	B	0.82	14/2482 (0.6%)	0.67	5/3329 (0.2%)
1	C	0.67	8/2528 (0.3%)	0.63	1/3391 (0.0%)
1	D	1.26	31/2432 (1.3%)	0.75	5/3261 (0.2%)
All	All	1.02	88/9895 (0.9%)	0.71	21/13270 (0.2%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	SER	CB-OG	-16.67	1.20	1.42
1	D	29	SER	CB-OG	-16.50	1.20	1.42
1	D	184	VAL	CB-CG2	-15.99	1.19	1.52
1	B	89	SER	CB-OG	-15.55	1.22	1.42
1	D	89	SER	C-O	-15.13	0.94	1.23
1	A	89	SER	C-O	-14.95	0.94	1.23
1	A	29	SER	CB-OG	-14.79	1.23	1.42
1	C	89	SER	CB-OG	-14.72	1.23	1.42
1	D	88	SER	C-O	-13.75	0.97	1.23
1	A	88	SER	CB-OG	-13.72	1.24	1.42
1	D	186	SER	CB-OG	-12.95	1.25	1.42
1	C	88	SER	CB-OG	-12.76	1.25	1.42
1	D	184	VAL	C-O	-12.57	0.99	1.23
1	A	33	GLY	C-O	-12.34	1.03	1.23
1	D	88	SER	CB-OG	-12.31	1.26	1.42
1	D	185	ARG	C-O	-12.06	1.00	1.23
1	B	89	SER	C-O	-11.24	1.01	1.23
1	B	88	SER	CB-OG	-11.23	1.27	1.42
1	A	89	SER	CB-OG	-11.22	1.27	1.42
1	A	88	SER	C-O	-11.20	1.02	1.23
1	D	28	LEU	C-O	-10.99	1.02	1.23
1	A	29	SER	C-O	-10.85	1.02	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	SER	C-O	-10.85	1.02	1.23
1	D	30	ALA	C-O	-10.67	1.03	1.23
1	A	90	GLU	CD-OE2	-10.17	1.14	1.25
1	B	90	GLU	CB-CG	-10.16	1.32	1.52
1	B	88	SER	C-O	-10.03	1.04	1.23
1	C	89	SER	C-O	-9.95	1.04	1.23
1	D	185	ARG	CZ-NH1	-9.81	1.20	1.33
1	B	165	LEU	C-O	-9.72	1.04	1.23
1	A	171	GLY	C-O	-9.41	1.08	1.23
1	C	90	GLU	CD-OE2	-9.22	1.15	1.25
1	A	27	ALA	C-O	-9.03	1.06	1.23
1	A	87	LEU	C-O	-9.03	1.06	1.23
1	D	90	GLU	CB-CG	-8.92	1.35	1.52
1	A	166	GLY	C-O	-8.90	1.09	1.23
1	A	30	ALA	C-O	-8.85	1.06	1.23
1	A	164	SER	CB-OG	-8.80	1.30	1.42
1	A	28	LEU	C-O	-8.66	1.06	1.23
1	D	87	LEU	CG-CD1	-8.12	1.21	1.51
1	D	31	THR	CB-CG2	-8.11	1.25	1.52
1	A	172	LEU	C-O	-7.89	1.08	1.23
1	D	185	ARG	CG-CD	-7.81	1.32	1.51
1	D	87	LEU	C-O	-7.78	1.08	1.23
1	D	87	LEU	CG-CD2	-7.71	1.23	1.51
1	D	29	SER	C-O	-7.65	1.08	1.23
1	A	90	GLU	C-O	-7.64	1.08	1.23
1	A	165	LEU	CG-CD1	-7.56	1.23	1.51
1	B	166	GLY	C-O	-7.42	1.11	1.23
1	A	31	THR	CB-CG2	-7.29	1.28	1.52
1	D	185	ARG	CZ-NH2	-7.26	1.23	1.33
1	D	27	ALA	C-O	-7.24	1.09	1.23
1	A	167	LEU	CG-CD2	-7.09	1.25	1.51
1	A	87	LEU	CG-CD1	-7.05	1.25	1.51
1	D	32	HIS	C-O	-7.05	1.09	1.23
1	C	90	GLU	CD-OE1	-7.03	1.18	1.25
1	D	28	LEU	CG-CD2	-6.96	1.26	1.51
1	A	165	LEU	C-O	-6.88	1.10	1.23
1	B	167	LEU	C-O	-6.80	1.10	1.23
1	A	87	LEU	CG-CD2	-6.74	1.26	1.51
1	A	164	SER	C-O	-6.72	1.10	1.23
1	A	32	HIS	C-O	-6.64	1.10	1.23
1	D	90	GLU	CD-OE1	-6.64	1.18	1.25
1	D	29	SER	N-CA	-6.62	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLY	N-CA	-6.57	1.36	1.46
1	A	90	GLU	CB-CG	-6.52	1.39	1.52
1	B	90	GLU	C-O	-6.33	1.11	1.23
1	D	29	SER	CA-CB	-6.25	1.43	1.52
1	A	169	LYS	N-CA	-6.12	1.34	1.46
1	A	31	THR	C-O	-6.02	1.11	1.23
1	C	90	GLU	C-O	-5.99	1.11	1.23
1	D	186	SER	N-CA	-5.90	1.34	1.46
1	D	30	ALA	CA-CB	-5.88	1.40	1.52
1	B	171	GLY	C-O	-5.74	1.14	1.23
1	D	31	THR	C-O	-5.62	1.12	1.23
1	A	29	SER	N-CA	-5.53	1.35	1.46
1	D	186	SER	C-O	-5.53	1.12	1.23
1	B	90	GLU	CD-OE2	-5.40	1.19	1.25
1	A	171	GLY	CA-C	-5.32	1.43	1.51
1	D	28	LEU	CG-CD1	-5.23	1.32	1.51
1	A	33	GLY	N-CA	-5.22	1.38	1.46
1	A	172	LEU	C-N	-5.22	1.22	1.34
1	A	30	ALA	N-CA	-5.17	1.36	1.46
1	A	29	SER	CA-CB	-5.13	1.45	1.52
1	B	169	LYS	N-CA	-5.08	1.36	1.46
1	A	28	LEU	CG-CD2	-5.07	1.33	1.51
1	B	165	LEU	CG-CD1	-5.05	1.33	1.51
1	C	89	SER	N-CA	-5.02	1.36	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	D	54	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	B	171	GLY	N-CA-C	8.63	134.67	113.10
1	B	128	ASP	N-CA-C	-7.55	90.62	111.00
1	B	165	LEU	CB-CG-CD1	-7.07	98.97	111.00
1	A	167	LEU	CA-CB-CG	6.79	130.91	115.30
1	C	149	ASN	N-CA-C	-6.31	93.97	111.00
1	D	185	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	D	185	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	167	LEU	O-C-N	-6.05	113.02	122.70
1	A	168	GLU	N-CA-CB	6.00	121.40	110.60
1	A	172	LEU	CB-CG-CD1	5.73	120.74	111.00
1	A	87	LEU	CB-CG-CD1	5.72	120.73	111.00
1	A	165	LEU	CB-CG-CD2	-5.66	101.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CD-CE-NZ	5.62	124.64	111.70
1	D	87	LEU	CB-CG-CD1	5.55	120.43	111.00
1	B	170	GLY	N-CA-C	5.45	126.72	113.10
1	A	170	GLY	N-CA-C	5.16	126.01	113.10
1	A	171	GLY	N-CA-C	-5.12	100.30	113.10
1	A	46	ARG	CB-CG-CD	5.09	124.83	111.60
1	B	169	LYS	CB-CA-C	-5.07	100.25	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2419	0	2472	57	0
1	B	2447	0	2482	66	0
1	C	2491	0	2530	62	0
1	D	2399	0	2446	56	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	174	0	0	4	0
3	B	153	0	0	7	0
3	C	168	0	0	8	0
3	D	180	0	0	4	0
All	All	10439	0	9930	233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (233) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:THR:H	1:A:135:MET:HE2	1.26	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:244:THR:HA	1:C:249:ARG:HD3	1.40	0.98
1:B:244:THR:HA	1:B:249:ARG:HD3	1.44	0.97
1:A:244:THR:HA	1:A:249:ARG:HD3	1.53	0.91
1:B:1:MET:HA	1:B:82:GLU:HG2	1.55	0.88
1:D:244:THR:HA	1:D:249:ARG:HD3	1.56	0.88
1:C:1:MET:HA	1:C:82:GLU:HG2	1.62	0.81
1:D:151:MET:CE	1:D:156:GLU:HA	2.13	0.78
1:A:143:ARG:HD3	3:A:718:HOH:O	1.84	0.77
1:A:311:ILE:HD12	1:A:311:ILE:H	1.50	0.76
1:C:151:MET:CB	1:C:155:GLU:HB2	2.18	0.74
1:D:156:GLU:O	1:D:160:GLN:HG2	1.90	0.72
1:A:22:ARG:HD3	1:A:23:ARG:N	2.06	0.70
1:C:145:ARG:HB3	1:C:151:MET:HE2	1.74	0.70
1:B:106:LYS:HD3	3:B:695:HOH:O	1.93	0.68
1:D:151:MET:HE3	1:D:156:GLU:HA	1.76	0.68
1:A:123:THR:N	1:A:135:MET:HE2	2.07	0.67
1:B:1:MET:HB2	1:B:83:PHE:O	1.94	0.67
1:C:27:ALA:O	1:C:31:THR:HG23	1.95	0.66
1:C:1:MET:HB2	1:C:83:PHE:O	1.95	0.66
1:C:151:MET:HB2	1:C:155:GLU:HB2	1.77	0.66
1:C:151:MET:HB3	1:C:155:GLU:HB2	1.78	0.65
1:C:21:VAL:HG21	1:C:89:SER:HB2	1.79	0.65
1:A:292:ASN:HB3	1:A:296:LYS:HZ3	1.62	0.64
1:A:167:LEU:O	1:A:170:GLY:N	2.30	0.64
1:B:152:SER:OG	1:B:155:GLU:HG3	1.98	0.63
1:D:80:LYS:HE2	3:D:755:HOH:O	1.98	0.63
1:D:145:ARG:O	1:D:146:SER:CB	2.47	0.62
1:B:154:SER:O	1:B:157:LYS:HG2	1.99	0.62
1:C:2:ILE:HD12	1:C:44:GLN:HB3	1.79	0.62
1:B:240:GLY:O	1:B:249:ARG:HD2	2.00	0.62
1:B:271:LYS:HD3	3:B:720:HOH:O	1.99	0.61
1:D:291:ASN:C	1:D:291:ASN:HD22	2.03	0.61
1:D:54:ARG:HB2	1:D:57:LYS:HB2	1.81	0.61
1:A:297:GLN:O	1:A:301:ILE:HG12	2.01	0.60
1:B:157:LYS:NZ	1:B:157:LYS:HB3	2.17	0.60
1:B:154:SER:HA	1:B:157:LYS:HE2	1.84	0.60
1:D:53:PHE:HB2	1:D:62:TYR:CE1	2.37	0.60
1:A:311:ILE:HD12	1:A:311:ILE:N	2.18	0.59
1:B:256:PHE:CE2	1:B:260:LYS:HD2	2.37	0.59
1:C:246:THR:HG22	1:C:281:GLU:O	2.02	0.59
1:B:151:MET:HB3	1:B:155:GLU:HB2	1.85	0.59
1:C:223:LEU:O	1:C:273:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:TYR:HE2	1:B:135:MET:HE2	1.69	0.58
1:C:256:PHE:CZ	1:C:260:LYS:HD2	2.38	0.58
1:A:53:PHE:HB2	1:A:62:TYR:CE1	2.39	0.58
1:A:271:LYS:HE3	1:A:308:SER:O	2.04	0.58
1:C:35:VAL:O	1:C:35:VAL:HG13	2.03	0.57
1:A:22:ARG:NH2	1:A:23:ARG:HG2	2.19	0.57
1:A:46:ARG:HG2	1:A:47:CYS:N	2.18	0.57
1:A:91:HIS:HE1	1:A:232:SER:OG	1.88	0.57
1:D:151:MET:HE2	1:D:156:GLU:HA	1.86	0.57
1:A:292:ASN:HB3	1:A:296:LYS:NZ	2.19	0.57
1:D:241:LYS:HE3	1:D:251:ASN:HD21	1.69	0.57
1:C:55:TYR:HE2	1:C:135:MET:HE2	1.70	0.57
1:C:91:HIS:HE1	1:C:232:SER:OG	1.87	0.57
1:A:152:SER:HB2	1:A:155:GLU:HG3	1.87	0.56
1:B:145:ARG:NH1	1:B:160:GLN:HE22	2.03	0.56
1:A:256:PHE:CZ	1:A:260:LYS:HD2	2.41	0.56
1:D:292:ASN:HD22	1:D:292:ASN:H	1.53	0.56
1:C:151:MET:HB3	1:C:155:GLU:OE1	2.06	0.56
1:D:292:ASN:HD22	1:D:292:ASN:N	2.03	0.55
1:B:271:LYS:NZ	1:B:271:LYS:HB2	2.21	0.55
1:C:1:MET:HE3	1:C:306:ILE:HG23	1.87	0.55
1:A:22:ARG:HH21	1:A:23:ARG:HG2	1.72	0.55
1:D:54:ARG:CB	1:D:57:LYS:HB2	2.36	0.55
1:B:256:PHE:CZ	1:B:260:LYS:HD2	2.41	0.55
1:D:115:LEU:HD12	1:D:115:LEU:N	2.21	0.55
1:D:33:GLY:HA2	1:D:42:ILE:HB	1.88	0.55
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.72	0.55
1:B:264:GLY:O	1:B:268:GLU:HG3	2.07	0.55
1:C:298:VAL:O	1:C:302:LEU:HD13	2.07	0.54
1:A:214:GLU:HG2	1:A:218:LYS:HE3	1.90	0.54
1:A:80:LYS:HE2	3:A:737:HOH:O	2.07	0.54
1:B:23:ARG:HH21	1:B:23:ARG:HG2	1.72	0.54
1:D:152:SER:OG	1:D:155:GLU:HG3	2.08	0.54
1:A:115:LEU:N	1:A:115:LEU:HD12	2.22	0.54
1:D:91:HIS:HE1	1:D:232:SER:OG	1.91	0.54
1:C:53:PHE:HB2	1:C:62:TYR:CE1	2.43	0.53
1:C:271:LYS:HE3	1:C:308:SER:O	2.09	0.53
1:B:1:MET:N	1:B:41:THR:O	2.41	0.53
1:B:53:PHE:HB2	1:B:62:TYR:CE1	2.43	0.53
1:B:291:ASN:H	1:B:291:ASN:HD22	1.56	0.53
1:D:145:ARG:O	1:D:145:ARG:HD3	2.09	0.53
1:A:54:ARG:HB2	1:A:57:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:GLU:O	1:A:156:GLU:HG2	2.09	0.53
1:D:292:ASN:ND2	1:D:292:ASN:H	2.06	0.53
1:C:28:LEU:HD11	1:C:302:LEU:HD23	1.91	0.53
1:A:160:GLN:O	1:A:164:SER:HB2	2.09	0.53
1:A:123:THR:H	1:A:135:MET:CE	2.10	0.52
1:A:51:LYS:HE2	1:A:61:ASP:HB3	1.91	0.52
1:D:6:LEU:HG	1:D:88:SER:HA	1.90	0.52
1:B:291:ASN:HD22	1:B:291:ASN:N	2.05	0.52
1:C:51:LYS:HE2	1:C:61:ASP:HB3	1.90	0.52
1:D:293:GLU:HA	1:D:296:LYS:HZ3	1.75	0.52
1:B:41:THR:HG21	1:B:306:ILE:CG2	2.40	0.52
1:C:145:ARG:HB3	1:C:151:MET:CE	2.39	0.51
1:B:51:LYS:HE2	1:B:61:ASP:HB3	1.91	0.51
1:A:221:GLU:O	1:A:224:LYS:HG2	2.11	0.51
1:C:271:LYS:HD3	3:C:760:HOH:O	2.09	0.51
1:B:54:ARG:CB	1:B:57:LYS:HB2	2.40	0.51
1:C:115:LEU:N	1:C:115:LEU:HD12	2.25	0.51
1:B:19:LYS:NZ	3:B:724:HOH:O	2.43	0.51
1:C:54:ARG:CB	1:C:57:LYS:HB2	2.40	0.51
1:D:145:ARG:O	1:D:146:SER:HB2	2.11	0.50
1:C:54:ARG:HB2	1:C:57:LYS:HB2	1.92	0.50
1:B:22:ARG:HH21	1:B:22:ARG:HG2	1.76	0.50
1:A:54:ARG:CB	1:A:57:LYS:HB2	2.42	0.50
1:C:240:GLY:O	1:C:249:ARG:HD2	2.12	0.50
1:B:223:LEU:O	1:B:273:ARG:NH2	2.45	0.50
1:B:54:ARG:HB2	1:B:57:LYS:HB2	1.92	0.50
1:D:51:LYS:HE2	1:D:61:ASP:HB3	1.93	0.50
1:C:54:ARG:HD3	3:C:637:HOH:O	2.12	0.50
1:B:115:LEU:HD12	1:B:115:LEU:N	2.26	0.50
1:A:202:LEU:HD23	1:A:202:LEU:C	2.32	0.49
1:A:244:THR:HG22	1:A:249:ARG:NH1	2.27	0.49
1:C:80:LYS:HE2	3:C:745:HOH:O	2.12	0.49
1:D:15:ARG:HD2	3:D:648:HOH:O	2.13	0.49
1:C:210:GLU:HG3	3:C:750:HOH:O	2.13	0.49
1:B:150:ARG:HA	1:B:150:ARG:HE	1.78	0.49
1:A:261:GLN:HE21	1:D:261:GLN:HE21	1.61	0.49
1:D:39:MET:HE2	3:D:728:HOH:O	2.12	0.49
1:D:1:MET:CA	1:D:82:GLU:HG2	2.42	0.48
1:C:67:LYS:HB2	1:C:165:LEU:HD22	1.96	0.48
1:A:19:LYS:HA	1:A:22:ARG:HG3	1.94	0.48
1:B:271:LYS:HE3	1:B:308:SER:O	2.13	0.48
1:B:291:ASN:ND2	1:B:291:ASN:N	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:35:VAL:HA	1:C:40:GLN:HB2	1.96	0.48
1:D:1:MET:HA	1:D:82:GLU:HG2	1.96	0.47
1:A:144:VAL:HG11	1:A:159:TRP:CD2	2.50	0.47
1:D:256:PHE:CZ	1:D:260:LYS:HD2	2.50	0.47
1:B:91:HIS:HE1	1:B:232:SER:OG	1.98	0.47
1:D:136:PRO:O	1:D:140:VAL:HG23	2.13	0.47
1:D:162:LEU:HD12	1:D:165:LEU:HD12	1.96	0.47
1:D:271:LYS:HE3	1:D:308:SER:O	2.15	0.46
1:A:36:ILE:HD12	1:B:199:GLN:HE22	1.81	0.46
1:C:231:LEU:HD23	1:C:231:LEU:C	2.35	0.46
1:B:293:GLU:O	1:B:297:GLN:HG3	2.15	0.46
1:B:63:TYR:CE1	1:B:165:LEU:HD21	2.51	0.46
1:B:268:GLU:HG2	3:B:718:HOH:O	2.16	0.46
1:B:109:LYS:HE2	3:B:706:HOH:O	2.14	0.46
1:B:242:LEU:HD23	3:B:701:HOH:O	2.16	0.46
1:B:125:TYR:CD1	1:B:131:HIS:HA	2.51	0.46
1:C:293:GLU:O	1:C:297:GLN:HG3	2.16	0.46
1:B:35:VAL:HA	1:B:40:GLN:HB2	1.98	0.46
1:B:157:LYS:HZ2	1:B:157:LYS:HB3	1.80	0.45
3:A:709:HOH:O	1:B:177:LYS:HB3	2.16	0.45
1:A:311:ILE:CD1	1:A:311:ILE:H	2.22	0.45
1:D:7:GLU:O	1:D:49:LEU:HA	2.16	0.45
1:C:125:TYR:CD1	1:C:131:HIS:HA	2.51	0.45
1:B:151:MET:HA	1:B:155:GLU:OE1	2.17	0.45
1:C:67:LYS:HB2	1:C:165:LEU:CD2	2.46	0.45
1:A:7:GLU:O	1:A:49:LEU:HA	2.16	0.45
1:B:71:ILE:HB	1:B:72:PRO:HD3	1.99	0.45
1:B:244:THR:HG21	1:B:288:ILE:HG12	1.99	0.45
1:D:292:ASN:ND2	1:D:292:ASN:N	2.65	0.45
1:A:1:MET:CA	1:A:82:GLU:HG2	2.46	0.45
1:B:310:LYS:O	1:B:311:ILE:HB	2.17	0.45
1:B:71:ILE:O	1:B:75:LYS:HG3	2.16	0.45
1:A:2:ILE:HG12	1:A:82:GLU:HB3	1.97	0.45
1:B:213:GLN:H	1:B:213:GLN:CD	2.20	0.45
1:C:7:GLU:O	1:C:49:LEU:HA	2.17	0.45
1:D:71:ILE:HB	1:D:72:PRO:HD3	1.98	0.45
1:B:244:THR:HG22	1:B:249:ARG:NH1	2.32	0.44
1:B:202:LEU:HD23	1:B:202:LEU:C	2.37	0.44
1:B:205:VAL:HG13	1:B:254:LEU:HD23	2.00	0.44
1:D:223:LEU:O	1:D:226:VAL:HG22	2.17	0.44
1:C:213:GLN:H	1:C:213:GLN:CD	2.21	0.44
1:D:145:ARG:HB3	1:D:151:MET:SD	2.58	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:GLN:HG3	1:D:261:GLN:CG	2.48	0.44
1:D:144:VAL:HG21	1:D:159:TRP:CE3	2.53	0.43
1:B:185:ARG:NH2	1:B:237:ILE:O	2.40	0.43
1:C:22:ARG:HH21	1:C:22:ARG:HG2	1.84	0.43
1:A:271:LYS:NZ	1:A:271:LYS:HB2	2.33	0.43
1:D:71:ILE:O	1:D:75:LYS:HG3	2.18	0.43
1:D:193:ASP:OD1	1:D:196:ARG:NH2	2.52	0.43
1:C:151:MET:HB3	1:C:155:GLU:CB	2.46	0.43
1:C:246:THR:CG2	1:C:281:GLU:O	2.65	0.43
1:A:121:ILE:O	1:A:138:GLY:HA3	2.18	0.43
1:C:71:ILE:HB	1:C:72:PRO:HD3	2.00	0.43
1:A:71:ILE:HB	1:A:72:PRO:HD3	1.99	0.43
1:A:33:GLY:HA2	1:A:42:ILE:HB	1.99	0.43
1:A:36:ILE:HD12	1:B:199:GLN:NE2	2.33	0.43
1:D:304:LEU:HD23	1:D:304:LEU:C	2.38	0.43
1:C:244:THR:HG21	1:C:288:ILE:HG12	2.01	0.43
1:C:60:GLU:OE1	1:C:60:GLU:HA	2.19	0.43
1:C:256:PHE:CE2	1:C:260:LYS:HD2	2.54	0.43
1:D:144:VAL:HG11	1:D:159:TRP:CD2	2.54	0.43
1:C:1:MET:N	1:C:41:THR:O	2.49	0.42
1:D:6:LEU:HD22	1:D:48:VAL:HB	2.01	0.42
1:A:263:LEU:O	1:A:267:LEU:HG	2.19	0.42
1:D:241:LYS:HG2	1:D:251:ASN:ND2	2.34	0.42
1:C:122:HIS:CE1	1:C:146:SER:HB3	2.55	0.42
1:A:160:GLN:NE2	1:A:160:GLN:C	2.73	0.42
1:C:202:LEU:HD23	1:C:202:LEU:C	2.40	0.42
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.87	0.42
1:D:231:LEU:HD23	1:D:231:LEU:C	2.39	0.42
1:D:242:LEU:HD23	1:D:255:SER:HA	2.01	0.42
1:D:199:GLN:NE2	3:D:661:HOH:O	2.51	0.42
1:D:296:LYS:O	1:D:300:GLU:HG3	2.20	0.42
1:A:71:ILE:O	1:A:75:LYS:HG3	2.19	0.42
1:A:244:THR:HG22	1:A:249:ARG:HH11	1.84	0.42
1:C:41:THR:HG21	1:C:306:ILE:CG2	2.50	0.42
1:B:23:ARG:NH2	1:B:23:ARG:HG2	2.33	0.42
1:B:60:GLU:OE1	1:B:60:GLU:HA	2.20	0.42
1:D:60:GLU:HA	1:D:60:GLU:OE1	2.20	0.42
1:C:251:ASN:ND2	3:C:685:HOH:O	2.53	0.41
1:C:71:ILE:O	1:C:75:LYS:HG3	2.20	0.41
1:C:304:LEU:HD23	1:C:304:LEU:O	2.19	0.41
1:A:160:GLN:NE2	3:A:747:HOH:O	2.52	0.41
1:B:231:LEU:HD23	1:B:231:LEU:C	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:GLU:O	1:B:49:LEU:HA	2.20	0.41
1:C:242:LEU:HD23	3:C:666:HOH:O	2.19	0.41
1:B:263:LEU:O	1:B:267:LEU:HG	2.20	0.41
1:B:307:ASN:O	1:B:310:LYS:HE2	2.21	0.41
1:C:201:PRO:HB3	1:D:37:LYS:HA	2.01	0.41
1:A:244:THR:HG21	1:A:288:ILE:HG12	2.01	0.41
1:B:145:ARG:CZ	1:B:160:GLN:HE22	2.33	0.41
1:B:210:GLU:HG3	3:B:702:HOH:O	2.21	0.41
1:D:206:ASP:O	1:D:210:GLU:HG3	2.20	0.41
1:D:239:ASP:HB3	1:D:242:LEU:HB2	2.01	0.41
1:C:109:LYS:HE2	3:C:668:HOH:O	2.20	0.41
1:A:22:ARG:HH21	1:A:23:ARG:CG	2.33	0.41
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.21	0.41
1:C:304:LEU:HD23	1:C:304:LEU:C	2.41	0.41
1:C:145:ARG:CB	1:C:151:MET:HE2	2.46	0.40
1:A:179:LEU:HD23	1:A:200:ILE:HD13	2.02	0.40
1:D:221:GLU:O	1:D:224:LYS:HG2	2.21	0.40
1:A:1:MET:HA	1:A:82:GLU:HG2	2.02	0.40
1:B:252:ASN:HB2	1:D:199:GLN:HE22	1.87	0.40
1:A:199:GLN:HE22	1:C:252:ASN:HB2	1.87	0.40
1:C:273:ARG:HD3	3:C:732:HOH:O	2.21	0.40
1:A:37:LYS:HA	1:B:201:PRO:HB3	2.02	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	295/330 (89%)	281 (95%)	14 (5%)	0	100	100
1	B	299/330 (91%)	287 (96%)	12 (4%)	0	100	100
1	C	306/330 (93%)	285 (93%)	20 (6%)	1 (0%)	50	53
1	D	294/330 (89%)	280 (95%)	14 (5%)	0	100	100
All	All	1194/1320 (90%)	1133 (95%)	60 (5%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	ARG

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	269/296 (91%)	259 (96%)	10 (4%)	45	54
1	B	273/296 (92%)	260 (95%)	13 (5%)	35	41
1	C	278/296 (94%)	261 (94%)	17 (6%)	26	28
1	D	267/296 (90%)	256 (96%)	11 (4%)	41	49
All	All	1087/1184 (92%)	1036 (95%)	51 (5%)	36	42

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	22	ARG
1	A	87	LEU
1	A	91	HIS
1	A	160	GLN
1	A	164	SER
1	A	271	LYS
1	A	272	ASP
1	A	292	ASN
1	A	302	LEU
1	B	91	HIS
1	B	129	SER
1	B	130	LYS
1	B	142	ASN
1	B	143	ARG
1	B	157	LYS
1	B	160	GLN
1	B	169	LYS
1	B	172	LEU
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	271	LYS
1	B	291	ASN
1	B	303	ASP
1	C	31	THR
1	C	37	LYS
1	C	91	HIS
1	C	130	LYS
1	C	142	ASN
1	C	145	ARG
1	C	146	SER
1	C	148	PHE
1	C	150	ARG
1	C	151	MET
1	C	152	SER
1	C	160	GLN
1	C	172	LEU
1	C	223	LEU
1	C	246	THR
1	C	271	LYS
1	C	293	GLU
1	D	6	LEU
1	D	15	ARG
1	D	22	ARG
1	D	91	HIS
1	D	142	ASN
1	D	145	ARG
1	D	265	LEU
1	D	271	LYS
1	D	291	ASN
1	D	292	ASN
1	D	302	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	44	GLN
1	A	91	HIS
1	A	160	GLN
1	A	199	GLN
1	A	251	ASN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	292	ASN
1	B	40	GLN
1	B	44	GLN
1	B	91	HIS
1	B	199	GLN
1	B	217	GLN
1	B	251	ASN
1	B	252	ASN
1	B	291	ASN
1	C	44	GLN
1	C	91	HIS
1	C	160	GLN
1	C	251	ASN
1	C	252	ASN
1	D	40	GLN
1	D	44	GLN
1	D	91	HIS
1	D	199	GLN
1	D	251	ASN
1	D	291	ASN
1	D	292	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

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	301/330 (91%)	-0.01	11 (3%)	39 40	15, 28, 69, 127	0
1	B	305/330 (92%)	0.18	22 (7%)	15 15	15, 31, 83, 118	1 (0%)
1	C	310/330 (93%)	0.09	19 (6%)	21 20	14, 28, 80, 130	1 (0%)
1	D	300/330 (90%)	-0.21	13 (4%)	34 34	14, 27, 70, 117	0
All	All	1216/1320 (92%)	0.01	65 (5%)	25 25	14, 28, 78, 130	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	PHE	7.5
1	D	55	TYR	5.3
1	A	55	TYR	5.1
1	C	290	HIS	4.7
1	A	125	TYR	4.5
1	C	37	LYS	4.4
1	D	145	ARG	4.4
1	B	33	GLY	3.9
1	A	168	GLU	3.9
1	C	36	ILE	3.9
1	B	290	HIS	3.9
1	A	124	ALA	3.9
1	B	129	SER	3.8
1	B	35	VAL	3.8
1	C	311	ILE	3.7
1	B	40	GLN	3.6
1	B	311	ILE	3.6
1	B	152	SER	3.6
1	B	150	ARG	3.6
1	C	129	SER	3.5
1	B	145	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	LYS	3.4
1	C	150	ARG	3.4
1	C	39	MET	3.4
1	B	151	MET	3.3
1	B	153	GLU	3.3
1	C	128	ASP	3.2
1	C	149	ASN	3.2
1	C	170	GLY	3.2
1	D	146	SER	3.1
1	C	168	GLU	3.1
1	B	170	GLY	3.0
1	C	57	LYS	2.9
1	B	34	ASP	2.9
1	A	290	HIS	2.8
1	B	154	SER	2.8
1	A	151	MET	2.8
1	C	151	MET	2.8
1	A	54	ARG	2.7
1	B	128	ASP	2.7
1	D	170	GLY	2.7
1	C	145	ARG	2.7
1	B	156	GLU	2.6
1	C	56	ALA	2.6
1	C	152	SER	2.6
1	D	124	ALA	2.6
1	D	54	ARG	2.6
1	B	57	LYS	2.5
1	A	288	ILE	2.4
1	A	57	LYS	2.3
1	B	56	ALA	2.3
1	D	57	LYS	2.3
1	C	169	LYS	2.3
1	B	168	GLU	2.2
1	B	106	LYS	2.2
1	B	291	ASN	2.2
1	D	159	TRP	2.1
1	C	35	VAL	2.1
1	A	159	TRP	2.1
1	D	157	LYS	2.1
1	D	169	LYS	2.0
1	A	132	ILE	2.0
1	D	81	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	154	SER	2.0
1	D	151	MET	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

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	C	501	1/1	0.17	2.61	25,25,25,25	0
2	MN	B	501	1/1	0.16	2.01	26,26,26,26	0
2	MN	A	501	1/1	0.12	0.33	28,28,28,28	0
2	MN	D	501	1/1	0.09	-0.98	24,24,24,24	0
2	MN	D	500	1/1	0.06	-2.64	34,34,34,34	0
2	MN	C	500	1/1	0.06	-2.89	37,37,37,37	0
2	MN	A	500	1/1	0.05	-3.13	32,32,32,32	0
2	MN	B	500	1/1	0.05	-3.51	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.