



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:40 AM GMT

PDB ID : 1G5H  
Title : CRYSTAL STRUCTURE OF THE ACCESSORY SUBUNIT OF MURINE  
MITOCHONDRIAL POLYMERASE GAMMA  
Authors : Carrodeguas, J.A.; Theis, K.; Bogenhagen, D.F.; Kisker, C.  
Deposited on : 2000-11-01  
Resolution : 1.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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

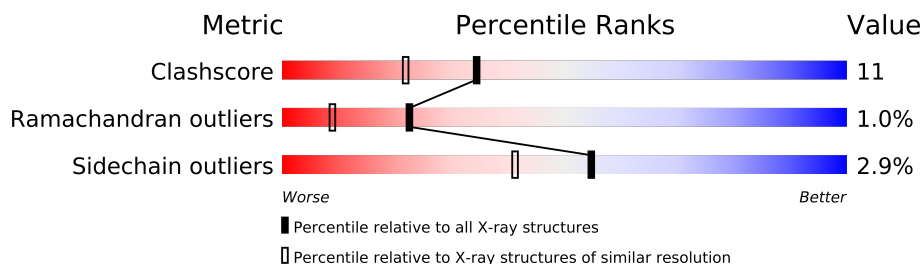
MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683



# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	
1	C	454	
1	D	454	



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13779 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 MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	Se	0	0	0
			3220	2050	570	586	8	6			
1	B	397	Total	C	N	O	S	Se	0	0	0
			3153	2010	554	575	8	6			
1	C	405	Total	C	N	O	S	Se	0	0	0
			3213	2045	568	586	8	6			
1	D	415	Total	C	N	O	S	Se	0	0	0
			3305	2103	587	601	8	6			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	409	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	436	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	439	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	440	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
A	460	ALA	-	EXPRESSION TAG	UNP Q9QZM2
A	461	ALA	-	EXPRESSION TAG	UNP Q9QZM2
A	462	ALA	-	EXPRESSION TAG	UNP Q9QZM2
A	463	LEU	-	EXPRESSION TAG	UNP Q9QZM2
A	464	ASP	-	EXPRESSION TAG	UNP Q9QZM2
A	465	HIS	-	EXPRESSION TAG	UNP Q9QZM2
A	466	HIS	-	EXPRESSION TAG	UNP Q9QZM2
A	467	HIS	-	EXPRESSION TAG	UNP Q9QZM2
A	468	HIS	-	EXPRESSION TAG	UNP Q9QZM2
A	469	HIS	-	EXPRESSION TAG	UNP Q9QZM2
A	470	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	92	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
B	409	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
B	439	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
B	440	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
B	460	ALA	-	EXPRESSION TAG	UNP Q9QZM2
B	461	ALA	-	EXPRESSION TAG	UNP Q9QZM2
B	462	ALA	-	EXPRESSION TAG	UNP Q9QZM2
B	463	LEU	-	EXPRESSION TAG	UNP Q9QZM2
B	464	ASP	-	EXPRESSION TAG	UNP Q9QZM2
B	465	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	466	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	467	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	468	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	469	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	470	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	92	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	242	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	409	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	436	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	439	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	440	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
C	460	ALA	-	EXPRESSION TAG	UNP Q9QZM2
C	461	ALA	-	EXPRESSION TAG	UNP Q9QZM2
C	462	ALA	-	EXPRESSION TAG	UNP Q9QZM2
C	463	LEU	-	EXPRESSION TAG	UNP Q9QZM2
C	464	ASP	-	EXPRESSION TAG	UNP Q9QZM2
C	465	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	466	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	467	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	468	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	469	HIS	-	EXPRESSION TAG	UNP Q9QZM2
C	470	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	92	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	242	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	409	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	436	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	439	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	440	MSE	MET	MODIFIED RESIDUE	UNP Q9QZM2
D	460	ALA	-	EXPRESSION TAG	UNP Q9QZM2
D	461	ALA	-	EXPRESSION TAG	UNP Q9QZM2
D	462	ALA	-	EXPRESSION TAG	UNP Q9QZM2
D	463	LEU	-	EXPRESSION TAG	UNP Q9QZM2
D	464	ASP	-	EXPRESSION TAG	UNP Q9QZM2

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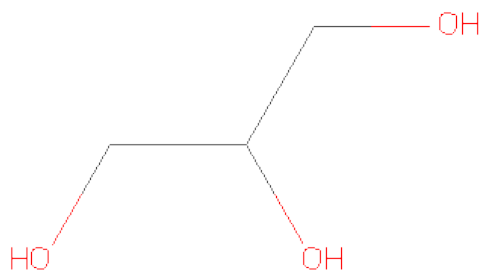
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Chain	Residue	Modelled	Actual	Comment	Reference
D	465	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	466	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	467	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	468	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	469	HIS	-	EXPRESSION TAG	UNP Q9QZM2
D	470	HIS	-	EXPRESSION TAG	UNP Q9QZM2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0



- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total 220	O 220	0	0
4	B	234	Total 234	O 234	0	0
4	C	214	Total 214	O 214	0	0
4	D	204	Total 204	O 204	0	0



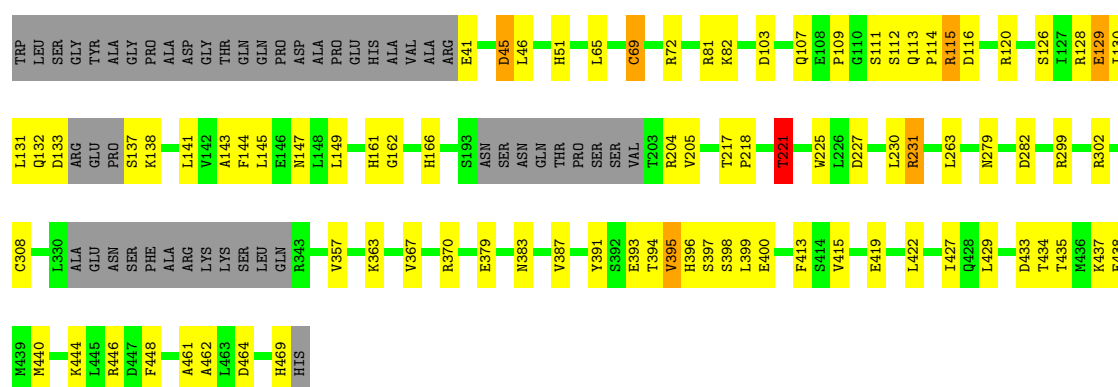
### 3 Residue-property plots

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.

Note EDS was not executed.

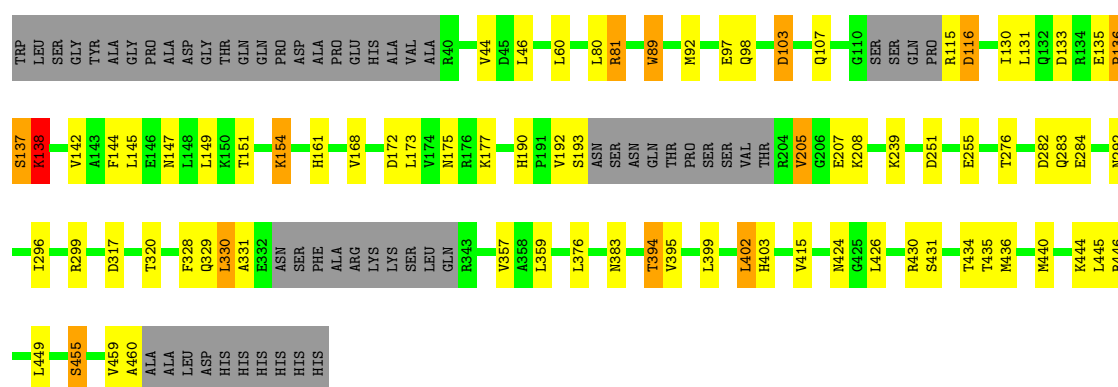
#### • Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain A:



#### • Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain B:



#### • Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain C:









## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.62Å 133.42Å 135.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	100.0 (20.00-1.95)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.183 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.81	0/3289	0.90	7/4447 (0.2%)
1	B	0.81	1/3217 (0.0%)	0.98	10/4348 (0.2%)
1	C	0.80	1/3281 (0.0%)	0.92	7/4436 (0.2%)
1	D	0.80	2/3375 (0.1%)	0.96	11/4561 (0.2%)
All	All	0.80	4/13162 (0.0%)	0.94	35/17792 (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	2
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	TYR	CD2-CE2	-5.64	1.30	1.39
1	D	73	PHE	CD2-CE2	5.24	1.49	1.39
1	B	89	TRP	CB-CG	-5.10	1.41	1.50
1	D	92	MSE	SE-CE	-5.08	1.65	1.95

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	ASP	CB-CG-OD2	11.39	128.55	118.30
1	B	81	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	B	81	ARG	NE-CZ-NH1	10.15	125.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	HIS	CA-CB-CG	-7.53	100.81	113.60
1	D	103	ASP	CB-CG-OD2	6.98	124.58	118.30
1	B	103	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	116	ASP	CB-CG-OD2	6.82	124.44	118.30
1	D	120	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	138	LYS	N-CA-C	-6.45	93.59	111.00
1	B	251	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	172	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	464	ASP	OD1-CG-OD2	-5.87	112.14	123.30
1	B	330	LEU	N-CA-C	-5.81	95.31	111.00
1	C	447	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	103	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	282	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	45	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	221	THR	N-CA-CB	-5.67	99.53	110.30
1	C	103	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	40	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	433	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	336	ALA	N-CA-C	5.47	125.77	111.00
1	C	133	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	120	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	227	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	433	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	40	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	227	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	116	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	172	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	133	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	282	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	161	HIS	CA-CB-CG	-5.21	104.74	113.60
1	D	135	GLU	N-CA-C	-5.21	96.93	111.00
1	D	315	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	468	HIS	Sidechain
1	C	469	HIS	Sidechain
1	D	466	HIS	Sidechain
1	D	468	HIS	Sidechain



## 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	3220	0	3206	81	0
1	B	3153	0	3154	86	0
1	C	3213	0	3194	67	0
1	D	3305	0	3300	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	6	0	8	1	0
3	D	6	0	8	0	0
4	A	220	0	0	5	0
4	B	234	0	0	9	0
4	C	214	0	0	4	0
4	D	204	0	0	5	0
All	All	13779	0	12870	277	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 11.

All (277) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:135:GLU:H	1:D:136:PRO:CD	1.36	1.26
1:D:134:ARG:HA	1:D:136:PRO:HD3	1.24	1.18
1:A:394:THR:O	1:A:395:VAL:HG22	1.01	1.17
1:A:394:THR:O	1:A:395:VAL:CG2	1.93	1.17
1:C:205:VAL:HG13	1:D:107:GLN:NE2	1.60	1.14
1:D:135:GLU:N	1:D:136:PRO:HD3	1.66	1.11
1:D:135:GLU:H	1:D:136:PRO:HD3	0.94	1.10
1:C:205:VAL:CG1	1:D:107:GLN:HE22	1.69	1.05
1:A:109:PRO:HG3	1:D:58:GLN:HE21	1.21	1.04
1:C:110:GLY:HA3	1:C:152:SER:O	1.63	0.98
1:A:114:PRO:O	1:A:115:ARG:HG2	1.64	0.98
1:B:383:ASN:HD21	1:B:446:ARG:HH21	1.14	0.95
1:B:115:ARG:CB	1:B:154:LYS:HE2	1.97	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:134:ARG:CA	1:D:136:PRO:HD3	1.96	0.95
1:C:205:VAL:HG13	1:D:107:GLN:HE22	0.80	0.93
1:D:135:GLU:N	1:D:136:PRO:CD	2.21	0.91
1:C:468:HIS:O	1:C:469:HIS:CB	2.19	0.89
1:B:383:ASN:HD21	1:B:446:ARG:NH2	1.69	0.89
1:A:112:SER:HB3	1:A:149:LEU:O	1.74	0.88
1:C:468:HIS:O	1:C:469:HIS:HB2	1.70	0.87
1:C:440:MSE:HE1	1:C:445:LEU:HA	1.56	0.86
1:C:467:HIS:CG	1:C:468:HIS:N	2.44	0.86
1:C:107:GLN:OE1	1:D:205:VAL:HG13	1.77	0.85
1:D:132:GLN:O	1:D:134:ARG:N	2.11	0.82
1:C:467:HIS:CG	1:C:468:HIS:H	1.98	0.82
1:C:137:SER:OG	1:C:140:GLN:NE2	2.13	0.81
1:A:114:PRO:O	1:A:115:ARG:CG	2.28	0.80
1:D:330:LEU:HD11	1:D:342:GLN:HB3	1.64	0.78
1:D:397:SER:OG	1:D:402:LEU:HD13	1.84	0.77
1:A:130:ILE:HD11	1:B:145:LEU:HD13	1.65	0.77
1:A:363:LYS:HA	1:A:363:LYS:HE2	1.66	0.77
1:D:117:SER:O	1:D:118:ALA:C	2.22	0.77
1:C:434:THR:O	1:C:435:THR:HB	1.83	0.77
1:B:81:ARG:HD2	4:B:919:HOH:O	1.85	0.77
1:B:115:ARG:HB3	1:B:154:LYS:HE2	1.66	0.76
1:D:134:ARG:HA	1:D:136:PRO:CD	2.13	0.75
1:C:113:GLN:H	1:C:114:PRO:HD2	1.51	0.75
1:B:460:ALA:HB2	4:B:1084:HOH:O	1.87	0.74
1:B:440:MSE:HE1	1:B:445:LEU:HA	1.69	0.73
1:B:190:HIS:CE1	1:B:208:LYS:HD3	2.25	0.70
1:D:440:MSE:HE3	1:D:444:LYS:HB2	1.72	0.70
1:C:110:GLY:CA	1:C:152:SER:O	2.41	0.69
1:B:440:MSE:HE3	1:B:444:LYS:CB	2.22	0.69
1:B:190:HIS:HE1	1:B:208:LYS:HD3	1.58	0.68
1:C:113:GLN:H	1:C:114:PRO:CD	2.06	0.68
1:B:283:GLN:HG3	4:B:997:HOH:O	1.92	0.67
1:B:328:PHE:CE2	1:B:330:LEU:HD11	2.29	0.67
1:B:161:HIS:ND1	4:B:977:HOH:O	2.26	0.67
1:D:383:ASN:HD21	1:D:446:ARG:HH21	1.43	0.67
1:C:442:ILE:O	1:C:442:ILE:HD13	1.97	0.65
1:B:435:THR:HG22	1:B:435:THR:O	1.97	0.65
1:B:434:THR:O	1:B:435:THR:HB	1.96	0.65
1:B:115:ARG:CA	1:B:154:LYS:HE2	2.26	0.64
1:A:221:THR:HG23	1:A:225:TRP:CD1	2.31	0.64
1:B:239:LYS:NZ	1:B:460:ALA:HB1	2.12	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:394:THR:C	1:A:395:VAL:HG22	2.07	0.64
1:C:162:GLY:O	1:C:166:HIS:HD2	1.81	0.64
1:A:129:GLU:OE1	1:A:130:ILE:HG23	1.98	0.63
1:A:41:GLU:HG3	1:A:45:ASP:OD2	1.98	0.63
1:A:383:ASN:HD21	1:A:446:ARG:CZ	2.12	0.63
1:C:205:VAL:CG1	1:D:107:GLN:NE2	2.42	0.63
1:D:134:ARG:C	1:D:136:PRO:HD3	2.20	0.62
1:A:128:ARG:HG3	1:B:149:LEU:HD21	1.81	0.62
1:A:107:GLN:HE22	1:B:205:VAL:HG22	1.62	0.62
1:D:204:ARG:NE	4:D:979:HOH:O	2.33	0.62
1:A:114:PRO:O	1:A:115:ARG:CB	2.47	0.62
1:B:440:MSE:HE1	1:B:445:LEU:N	2.14	0.62
1:B:440:MSE:HE1	1:B:445:LEU:CA	2.29	0.62
1:A:112:SER:CB	1:A:149:LEU:O	2.46	0.61
1:D:440:MSE:CE	1:D:444:LYS:HB2	2.30	0.61
1:B:440:MSE:HE3	1:B:444:LYS:HB3	1.82	0.60
1:B:192:VAL:O	1:B:193:SER:HB2	2.01	0.60
1:A:107:GLN:OE1	1:B:205:VAL:HG13	2.03	0.59
1:B:136:PRO:HG2	1:B:137:SER:H	1.68	0.59
1:A:162:GLY:O	1:A:166:HIS:HD2	1.86	0.59
1:A:440:MSE:HE1	1:A:448:PHE:CG	2.38	0.58
1:B:190:HIS:CE1	1:B:208:LYS:CD	2.86	0.58
1:B:434:THR:HB	1:B:436:MSE:HE3	1.85	0.58
1:B:430:ARG:NH2	1:B:435:THR:HG23	2.19	0.58
1:B:440:MSE:HE3	1:B:444:LYS:HB2	1.85	0.58
1:B:115:ARG:HA	1:B:154:LYS:HE2	1.85	0.58
1:D:332:GLU:HG2	1:D:342:GLN:HG2	1.85	0.58
1:A:130:ILE:HD11	1:B:145:LEU:CD1	2.32	0.58
1:A:138:LYS:HG3	1:B:136:PRO:CB	2.34	0.58
1:D:467:HIS:O	1:D:468:HIS:C	2.43	0.58
4:A:1111:HOH:O	1:B:97:GLU:HG3	2.04	0.57
1:C:108:GLU:OE1	1:C:154:LYS:NZ	2.36	0.57
1:D:162:GLY:O	1:D:166:HIS:HD2	1.88	0.57
1:C:65:LEU:O	1:C:72:ARG:HD3	2.04	0.57
1:D:89:TRP:HZ2	1:D:101:ALA:HB2	1.69	0.57
1:D:41:GLU:CD	1:D:43:LEU:H	2.08	0.57
1:C:329:GLN:HG3	4:C:1106:HOH:O	2.04	0.57
1:A:469:HIS:CD2	4:A:1065:HOH:O	2.57	0.57
1:C:468:HIS:O	1:C:469:HIS:HB3	2.05	0.57
1:D:424:ASN:OD1	1:D:424:ASN:O	2.23	0.56
1:D:362:GLY:HA3	1:D:418:THR:HG22	1.87	0.56
1:A:367:VAL:O	1:A:367:VAL:HG12	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:116:ASP:O	1:C:117:SER:CB	2.53	0.56
1:B:430:ARG:HH21	1:B:435:THR:HG23	1.70	0.56
1:A:113:GLN:N	1:A:114:PRO:CD	2.68	0.56
1:A:398:SER:HG	1:A:400:GLU:CD	2.08	0.56
1:D:383:ASN:HD21	1:D:446:ARG:NH2	2.02	0.56
1:A:379:GLU:HG2	1:A:446:ARG:HD2	1.88	0.56
1:A:299:ARG:HH22	1:B:394:THR:HB	1.71	0.56
1:D:46:LEU:HD23	1:D:46:LEU:C	2.26	0.56
1:A:393:GLU:CD	1:B:175:ASN:HD22	2.08	0.55
1:D:89:TRP:CZ2	1:D:101:ALA:HB2	2.41	0.55
1:B:168:VAL:CG2	1:B:296:ILE:HG22	2.36	0.55
1:A:398:SER:OG	1:A:400:GLU:OE1	2.17	0.55
1:D:440:MSE:HE1	1:D:444:LYS:C	2.27	0.55
1:C:283:GLN:HG3	4:C:951:HOH:O	2.07	0.55
1:B:115:ARG:CB	1:B:154:LYS:CE	2.80	0.54
1:C:363:LYS:HE2	4:C:1101:HOH:O	2.08	0.54
1:A:395:VAL:O	1:A:397:SER:N	2.40	0.54
1:A:132:GLN:O	1:A:133:ASP:CG	2.46	0.54
1:A:440:MSE:HE1	1:A:448:PHE:CB	2.38	0.54
1:B:394:THR:HG22	1:B:395:VAL:N	2.22	0.54
1:D:164:LEU:HD22	1:D:285:LEU:HD13	1.89	0.54
1:C:95:PHE:O	1:C:465:HIS:HE1	1.91	0.54
1:B:239:LYS:HZ2	1:B:460:ALA:HB1	1.73	0.53
1:B:276:THR:HG23	4:B:1040:HOH:O	2.08	0.53
1:C:434:THR:O	1:C:435:THR:CB	2.53	0.53
1:C:138:LYS:HD2	4:D:1068:HOH:O	2.08	0.53
1:B:115:ARG:HB2	1:B:154:LYS:HE2	1.90	0.53
1:D:376:LEU:HD21	1:D:445:LEU:HD23	1.92	0.52
1:D:336:ALA:C	1:D:337:ARG:HG2	2.29	0.52
1:A:400:GLU:CD	1:A:400:GLU:H	2.13	0.52
1:A:400:GLU:HG3	4:A:1113:HOH:O	2.09	0.52
1:A:221:THR:HG23	1:A:225:TRP:HD1	1.73	0.52
1:A:138:LYS:HD2	1:B:136:PRO:HG3	1.92	0.52
1:A:221:THR:HG21	4:A:921:HOH:O	2.09	0.52
1:D:69:CYS:SG	1:D:204:ARG:CG	2.98	0.52
1:D:383:ASN:ND2	1:D:446:ARG:HE	2.07	0.52
1:A:112:SER:HA	1:A:120:ARG:NH2	2.25	0.51
1:B:98:GLN:HB2	4:B:1091:HOH:O	2.10	0.51
1:C:376:LEU:HD11	1:C:445:LEU:HD23	1.93	0.51
1:D:168:VAL:HG23	1:D:289:TYR:CZ	2.45	0.51
1:C:92:MSE:SE	1:C:213:LEU:HD22	2.61	0.51
1:D:176:ARG:HB2	1:D:299:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:49:ARG:NH1	1:C:408:GLU:OE1	2.43	0.51
1:B:329:GLN:C	1:B:331:ALA:H	2.14	0.51
1:B:376:LEU:HD11	1:B:445:LEU:HD23	1.93	0.51
1:C:96:ARG:NH2	1:C:464:ASP:O	2.44	0.51
1:B:440:MSE:CE	1:B:445:LEU:N	2.73	0.51
1:A:126:SER:O	1:A:129:GLU:OE1	2.29	0.50
1:A:107:GLN:HG2	1:B:207:GLU:OE2	2.11	0.50
1:C:116:ASP:O	1:C:117:SER:HB2	2.11	0.50
1:B:284:GLU:HB2	4:B:971:HOH:O	2.11	0.50
1:A:217:THR:OG1	1:A:218:PRO:HD2	2.12	0.50
1:A:370:ARG:NH1	1:A:391:TYR:O	2.45	0.50
1:D:397:SER:OG	1:D:402:LEU:CD1	2.58	0.49
1:A:138:LYS:CD	1:B:136:PRO:HG3	2.42	0.49
1:D:121:LEU:HD12	1:D:121:LEU:N	2.27	0.49
1:D:228:PHE:O	1:D:231:ARG:HG2	2.11	0.49
1:A:231:ARG:NE	1:A:231:ARG:HA	2.27	0.49
1:C:137:SER:HG	1:C:140:GLN:NE2	2.08	0.49
1:A:394:THR:O	1:A:395:VAL:CB	2.58	0.48
1:C:46:LEU:C	1:C:46:LEU:HD23	2.33	0.48
1:A:144:PHE:HA	1:A:147:ASN:HD22	1.77	0.48
1:A:69:CYS:SG	1:A:204:ARG:HB3	2.53	0.48
1:B:440:MSE:HE1	1:B:444:LYS:C	2.34	0.48
1:A:113:GLN:HB2	1:A:114:PRO:HD3	1.95	0.48
1:C:467:HIS:CD2	1:C:468:HIS:N	2.81	0.48
1:C:465:HIS:HD2	1:D:382:GLU:OE2	1.97	0.48
1:A:82:LYS:HE2	1:B:89:TRP:CD1	2.48	0.48
1:A:415:VAL:HG13	1:A:427:ILE:HD12	1.96	0.48
1:B:359:LEU:HD23	1:B:415:VAL:HB	1.96	0.47
1:C:363:LYS:HD2	1:C:419:GLU:HB2	1.96	0.47
1:C:107:GLN:OE1	1:D:205:VAL:CG1	2.56	0.47
1:B:434:THR:O	1:B:435:THR:CB	2.61	0.47
1:A:231:ARG:HA	1:A:231:ARG:HE	1.79	0.47
1:C:90:SER:HA	1:C:94:VAL:HB	1.95	0.47
1:B:136:PRO:O	1:B:137:SER:CB	2.63	0.47
1:D:132:GLN:C	1:D:134:ARG:N	2.65	0.47
1:A:395:VAL:C	1:A:397:SER:H	2.17	0.47
1:D:69:CYS:SG	1:D:204:ARG:HB3	2.55	0.47
1:B:329:GLN:C	1:B:331:ALA:N	2.69	0.47
1:B:317:ASP:OD2	3:B:6:GOL:H11	2.15	0.47
1:C:205:VAL:CG1	1:D:107:GLN:OE1	2.63	0.46
1:A:143:ALA:O	1:A:147:ASN:ND2	2.49	0.46
1:D:356:LYS:HG2	1:D:386:SER:OG	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:ASN:OD1	1:A:308:CYS:SG	2.73	0.46
1:C:110:GLY:HA3	1:C:152:SER:C	2.34	0.46
1:D:205:VAL:HG13	4:D:971:HOH:O	2.15	0.46
1:B:136:PRO:HG2	1:B:137:SER:N	2.31	0.46
1:C:300:ASP:O	1:C:303:LYS:HE3	2.16	0.46
1:A:131:LEU:HD11	1:B:142:VAL:HG13	1.97	0.46
1:D:41:GLU:OE1	1:D:43:LEU:N	2.49	0.45
1:C:112:SER:HB3	1:C:149:LEU:O	2.17	0.45
1:C:253:GLN:HA	1:C:258:ARG:O	2.16	0.45
1:A:65:LEU:O	1:A:72:ARG:HD3	2.16	0.45
1:A:444:LYS:HG2	4:A:1071:HOH:O	2.16	0.45
1:C:419:GLU:O	1:C:422:LEU:HB2	2.17	0.45
1:B:357:VAL:HG21	1:B:449:LEU:HD13	1.97	0.45
1:D:82:LYS:NZ	4:D:1084:HOH:O	2.45	0.45
1:C:168:VAL:HG23	1:C:289:TYR:CZ	2.52	0.45
1:A:111:SER:OG	1:A:112:SER:N	2.50	0.44
1:B:130:ILE:HG13	1:B:144:PHE:CD1	2.53	0.44
1:C:411:VAL:O	1:C:432:ARG:HB2	2.16	0.44
1:A:394:THR:C	1:A:395:VAL:HG13	2.37	0.44
1:C:299:ARG:NH2	1:D:394:THR:OG1	2.49	0.44
1:B:455:SER:O	1:B:459:VAL:HG23	2.18	0.44
1:C:363:LYS:HG3	1:C:418:THR:HB	1.98	0.44
1:B:80:LEU:HG	1:B:320:THR:HG23	2.00	0.44
1:A:46:LEU:C	1:A:46:LEU:HD23	2.38	0.44
1:D:190:HIS:O	1:D:190:HIS:CD2	2.71	0.44
1:A:129:GLU:OE1	1:A:130:ILE:CG2	2.65	0.43
1:D:461:ALA:O	1:D:464:ASP:HB2	2.18	0.43
1:B:434:THR:HB	1:B:436:MSE:CE	2.46	0.43
1:B:135:GLU:HG3	1:B:136:PRO:HD2	2.00	0.43
1:D:147:ASN:HB3	4:D:1050:HOH:O	2.18	0.43
1:A:363:LYS:HA	1:A:363:LYS:CE	2.44	0.43
1:C:435:THR:O	1:C:435:THR:HG22	2.18	0.43
1:C:359:LEU:HD23	1:C:415:VAL:HB	2.01	0.43
1:D:110:GLY:HA3	1:D:152:SER:O	2.19	0.43
1:B:402:LEU:HA	1:B:402:LEU:HD12	1.86	0.43
1:B:46:LEU:HD23	1:B:46:LEU:C	2.39	0.43
1:A:413:PHE:HB3	1:A:429:LEU:HD11	2.00	0.43
1:A:461:ALA:O	1:A:462:ALA:C	2.57	0.43
1:B:115:ARG:HB2	1:B:154:LYS:CE	2.48	0.43
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.84	0.43
1:A:299:ARG:HH22	1:B:394:THR:CB	2.32	0.42
1:C:56:THR:HB	1:C:57:PRO:HD2	1.99	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:92:MSE:O	1:D:99:VAL:HG11	2.19	0.42
1:A:112:SER:CA	1:A:120:ARG:HH21	2.32	0.42
1:B:239:LYS:NZ	4:B:952:HOH:O	2.52	0.42
1:B:299:ARG:HG2	4:B:1122:HOH:O	2.18	0.42
1:C:440:MSE:CE	1:C:445:LEU:HA	2.37	0.42
1:A:137:SER:O	1:A:141:LEU:HG	2.19	0.42
1:D:378:ASN:O	1:D:382:GLU:HG3	2.19	0.42
1:D:190:HIS:HA	1:D:191:PRO:HD2	1.87	0.42
1:B:424:ASN:ND2	1:B:426:LEU:HG	2.34	0.42
1:B:383:ASN:ND2	1:B:446:ARG:HH21	1.97	0.42
1:A:434:THR:O	1:A:435:THR:OG1	2.24	0.42
1:A:399:LEU:HD23	1:A:437:LYS:NZ	2.34	0.42
1:A:137:SER:OG	1:A:138:LYS:N	2.51	0.42
1:C:161:HIS:O	1:C:165:GLU:HG3	2.19	0.42
1:B:44:VAL:HG11	1:B:60:LEU:HB3	2.02	0.42
1:B:136:PRO:CG	1:B:137:SER:N	2.81	0.42
1:D:41:GLU:OE1	1:D:43:LEU:HB3	2.20	0.42
1:D:227:ASP:CG	1:D:231:ARG:HH21	2.23	0.42
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.80	0.42
1:A:379:GLU:OE2	1:A:446:ARG:HD3	2.20	0.42
1:A:230:LEU:CD1	1:A:263:LEU:HD21	2.50	0.42
1:C:110:GLY:CA	1:C:153:GLY:HA2	2.49	0.41
1:A:81:ARG:HH22	1:B:103:ASP:CG	2.24	0.41
1:A:383:ASN:OD1	1:A:446:ARG:NE	2.53	0.41
1:A:419:GLU:O	1:A:422:LEU:HB2	2.20	0.41
1:A:398:SER:OG	1:A:400:GLU:CD	2.57	0.41
1:D:415:VAL:HG21	1:D:445:LEU:HD21	2.01	0.41
1:D:330:LEU:HD13	1:D:344:LYS:HG2	2.01	0.41
1:B:138:LYS:O	1:B:142:VAL:HB	2.20	0.41
1:A:145:LEU:HD13	1:B:130:ILE:HG21	2.02	0.41
1:C:357:VAL:HG21	1:C:449:LEU:HD13	2.01	0.41
1:B:399:LEU:HG	1:B:403:HIS:CE1	2.55	0.41
1:C:112:SER:HB3	1:C:120:ARG:HH21	1.86	0.41
1:A:51:HIS:CD2	1:B:173:LEU:HB2	2.55	0.41
1:A:367:VAL:O	1:A:367:VAL:CG1	2.69	0.41
1:C:377:LEU:HD12	1:C:387:VAL:HG11	2.02	0.41
1:B:424:ASN:OD1	1:B:424:ASN:C	2.59	0.41
1:C:68:GLY:HA2	4:C:974:HOH:O	2.21	0.41
1:D:65:LEU:O	1:D:72:ARG:HD3	2.21	0.41
1:C:426:LEU:HA	1:C:440:MSE:O	2.20	0.41
1:D:383:ASN:HD21	1:D:446:ARG:HE	1.68	0.41
1:C:112:SER:OG	1:C:150:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.87	0.41
1:B:147:ASN:O	1:B:151:THR:OG1	2.32	0.41
1:D:357:VAL:HA	1:D:413:PHE:O	2.21	0.41
1:C:363:LYS:CD	1:C:418:THR:HB	2.52	0.40
1:B:190:HIS:HE1	1:B:208:LYS:CD	2.27	0.40
1:B:135:GLU:HA	1:B:136:PRO:HD2	1.92	0.40
1:C:230:LEU:CD1	1:C:263:LEU:HD21	2.52	0.40
1:B:383:ASN:HD21	1:B:446:ARG:CZ	2.27	0.40
1:C:113:GLN:N	1:C:114:PRO:CD	2.75	0.40
1:D:440:MSE:HB3	1:D:440:MSE:HE2	1.93	0.40
1:D:69:CYS:SG	1:D:204:ARG:HG3	2.62	0.40
1:A:357:VAL:CG1	1:A:387:VAL:HG22	2.51	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	397/454 (87%)	383 (96%)	10 (2%)	4 (1%)	22	9
1	B	389/454 (86%)	378 (97%)	6 (2%)	5 (1%)	18	5
1	C	397/454 (87%)	385 (97%)	9 (2%)	3 (1%)	27	12
1	D	409/454 (90%)	387 (95%)	18 (4%)	4 (1%)	22	9
All	All	1592/1816 (88%)	1533 (96%)	43 (3%)	16 (1%)	22	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ASP
1	A	395	VAL
1	B	116	ASP
1	B	137	SER
1	B	138	LYS
1	C	363	LYS

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Mol	Chain	Res	Type
1	D	133	ASP
1	D	135	GLU
1	D	336	ALA
1	A	396	HIS
1	B	136	PRO
1	A	115	ARG
1	B	292	ASN
1	D	366	THR
1	C	113	GLN
1	C	114	PRO

### 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	357/391 (91%)	349 (98%)	8 (2%)	64	55
1	B	349/391 (89%)	338 (97%)	11 (3%)	51	37
1	C	355/391 (91%)	343 (97%)	12 (3%)	49	34
1	D	365/391 (93%)	354 (97%)	11 (3%)	53	39
All	All	1426/1564 (91%)	1384 (97%)	42 (3%)	55	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	129	GLU
1	A	205	VAL
1	A	221	THR
1	A	231	ARG
1	A	302	ARG
1	A	438	GLU
1	A	464	ASP
1	B	92	MSE
1	B	107	GLN
1	B	131	LEU
1	B	154	LYS

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Mol	Chain	Res	Type
1	B	177	LYS
1	B	205	VAL
1	B	255	GLU
1	B	394	THR
1	B	402	LEU
1	B	431	SER
1	B	455	SER
1	C	49	ARG
1	C	96	ARG
1	C	117	SER
1	C	231	ARG
1	C	329	GLN
1	C	392	SER
1	C	431	SER
1	C	438	GLU
1	C	442	ILE
1	C	446	ARG
1	C	464	ASP
1	C	468	HIS
1	D	92	MSE
1	D	98	GLN
1	D	116	ASP
1	D	131	LEU
1	D	135	GLU
1	D	205	VAL
1	D	244	PRO
1	D	292	ASN
1	D	303	LYS
1	D	402	LEU
1	D	446	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	166	HIS
1	A	374	GLN
1	A	403	HIS
1	A	428	GLN
1	B	58	GLN
1	B	175	ASN
1	B	190	HIS

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Mol	Chain	Res	Type
1	B	371	GLN
1	B	383	ASN
1	B	403	HIS
1	B	428	GLN
1	C	140	GLN
1	C	166	HIS
1	C	465	HIS
1	D	58	GLN
1	D	98	GLN
1	D	107	GLN
1	D	166	HIS
1	D	232	HIS
1	D	349	HIS
1	D	383	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	B	6	-	5,5,5	0.37	0	5,5,5	0.75	0
3	GOL	D	5	-	5,5,5	0.46	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	6	-	-	0/4/4/4	0/0/0/0
3	GOL	D	5	-	-	0/4/4/4	0/0/0/0

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.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.