



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:11 PM UTC

PDB ID : 1G5H / pdb_00001g5h
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 X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

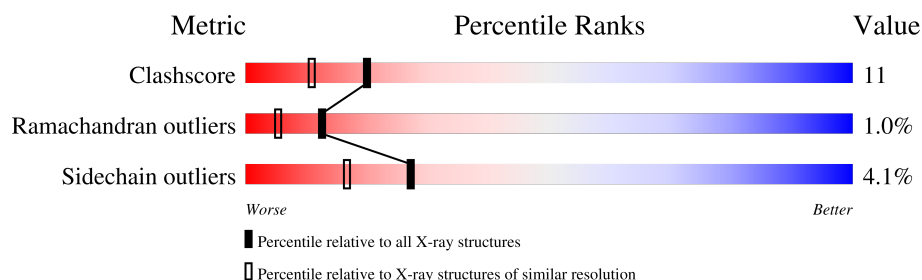
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	 68% 18% • 11%
1	B	454	 68% 16% • • 13%
1	C	454	 69% 16% • 11%
1	D	454	 71% 18% • • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13779 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 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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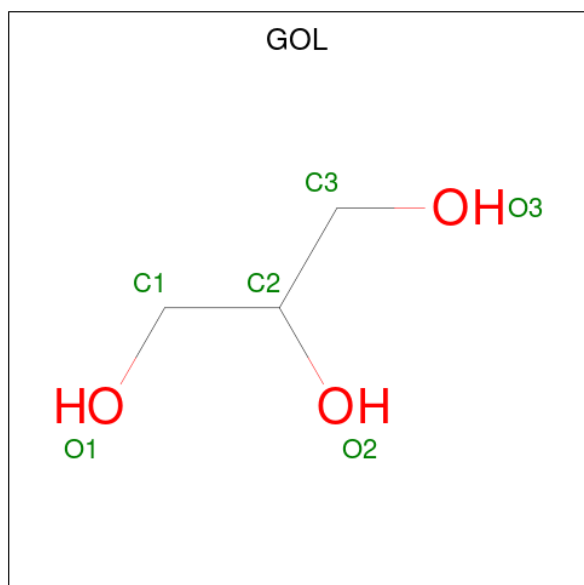
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Chain	Residue	Modelled	Actual	Comment	Reference
D	465	HIS	-	expression tag	UNP Q9QZM2
D	466	HIS	-	expression tag	UNP Q9QZM2
D	467	HIS	-	expression tag	UNP Q9QZM2
D	468	HIS	-	expression tag	UNP Q9QZM2
D	469	HIS	-	expression tag	UNP Q9QZM2
D	470	HIS	-	expression tag	UNP Q9QZM2

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

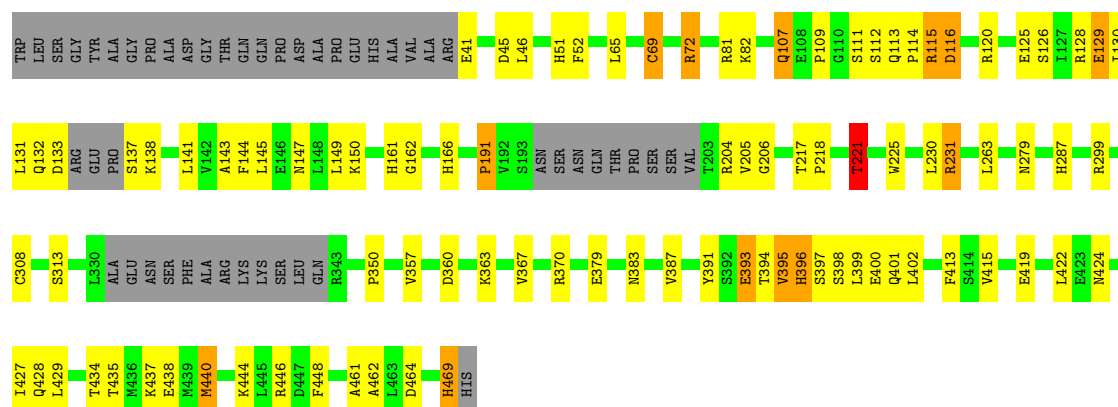
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

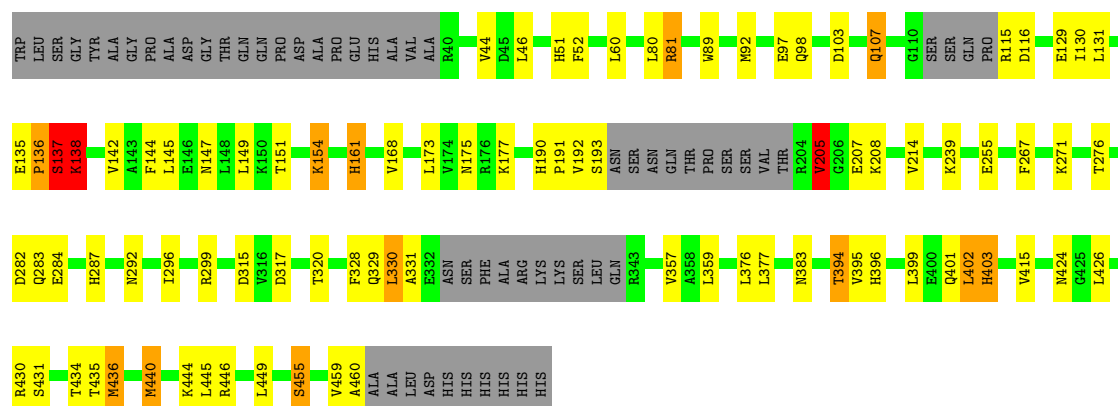
• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain A: 



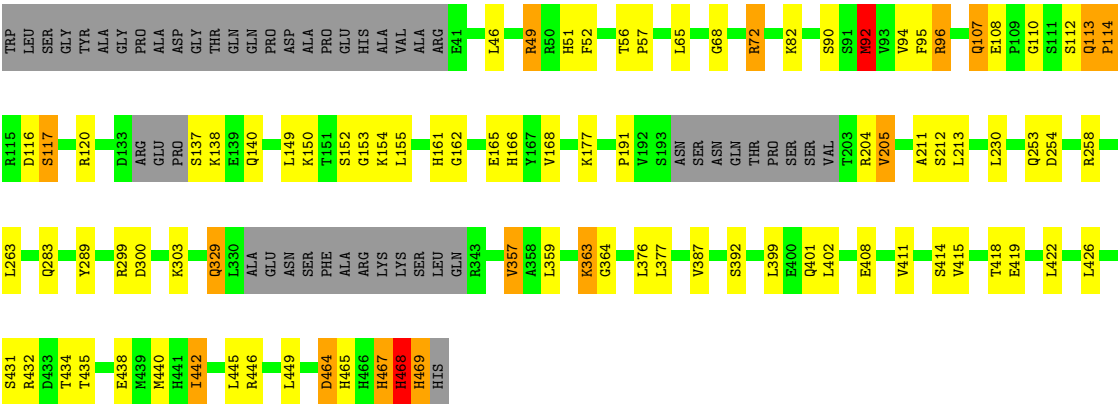
• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain B: 

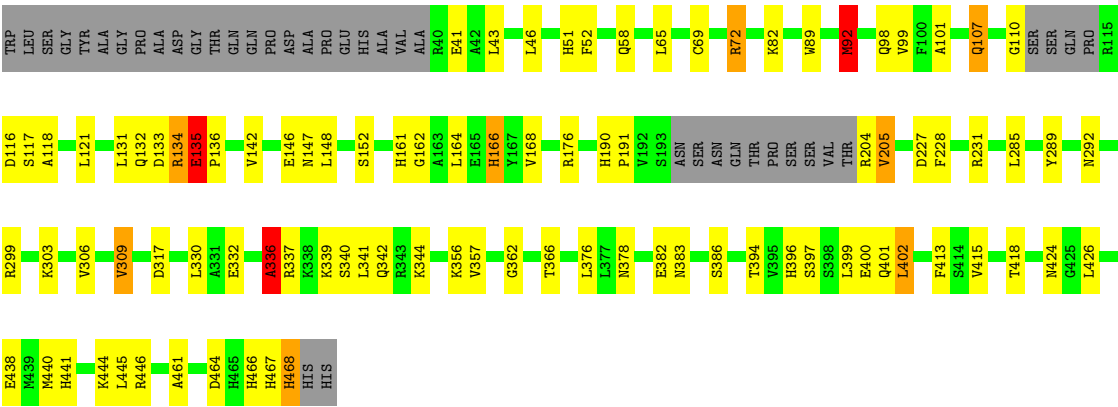


• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

Chain C: 



● Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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	Depositor
R, R_{free}	0.183 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13779	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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: 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	1.05	1/3289 (0.0%)	1.14	16/4447 (0.4%)
1	B	1.05	3/3217 (0.1%)	1.19	15/4348 (0.3%)
1	C	1.04	2/3281 (0.1%)	1.11	13/4436 (0.3%)
1	D	1.03	2/3375 (0.1%)	1.20	19/4561 (0.4%)
All	All	1.04	8/13162 (0.1%)	1.16	63/17792 (0.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	MSE	SE-CE	-9.98	1.65	1.95
1	C	92	MSE	SE-CE	-9.52	1.66	1.95
1	C	211	ALA	CA-CB	-7.86	1.43	1.53
1	B	214	VAL	CA-CB	-6.28	1.46	1.54
1	D	309	VAL	CA-CB	5.30	1.60	1.54
1	B	267	PHE	CA-C	5.26	1.59	1.52
1	B	330	LEU	CA-C	-5.25	1.47	1.53
1	A	206	GLY	CA-C	5.22	1.55	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	HIS	CA-CB-CG	-12.99	100.81	113.80
1	B	330	LEU	N-CA-C	-11.05	95.31	110.68
1	B	401	GLN	OE1-CD-NE2	-10.28	112.32	122.60
1	B	107	GLN	OE1-CD-NE2	-10.18	112.42	122.60
1	D	107	GLN	OE1-CD-NE2	-10.18	112.42	122.60
1	C	107	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	C	401	GLN	OE1-CD-NE2	-10.05	112.55	122.60
1	A	107	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	401	GLN	OE1-CD-NE2	-9.50	113.10	122.60
1	A	161	HIS	CA-CB-CG	-9.06	104.74	113.80
1	D	401	GLN	OE1-CD-NE2	-8.83	113.77	122.60
1	B	287	HIS	CA-CB-CG	-8.67	105.13	113.80
1	C	467	HIS	N-CA-C	8.54	122.25	109.95
1	B	138	LYS	N-CA-C	-8.08	93.59	110.80
1	A	396	HIS	CA-CB-CG	-7.70	106.10	113.80
1	D	441	HIS	CA-CB-CG	-7.63	106.17	113.80
1	D	166	HIS	CA-CB-CG	-7.57	106.23	113.80
1	A	221	THR	N-CA-CB	-7.57	99.53	110.80
1	B	161	HIS	CA-CB-CG	-7.49	106.31	113.80
1	B	191	PRO	CB-CA-C	7.41	121.05	111.64
1	C	52	PHE	N-CA-C	-7.12	102.93	111.69
1	D	336	ALA	N-CA-C	7.03	125.77	110.80
1	B	107	GLN	CG-CD-NE2	6.92	126.78	116.40
1	C	401	GLN	CG-CD-NE2	6.91	126.77	116.40
1	D	107	GLN	CG-CD-NE2	6.91	126.76	116.40
1	D	72	ARG	N-CA-C	6.90	120.96	112.54
1	D	52	PHE	N-CA-C	-6.76	103.06	112.45
1	B	396	HIS	CA-CB-CG	-6.74	107.06	113.80
1	A	401	GLN	CG-CD-NE2	6.69	126.44	116.40
1	A	107	GLN	CG-CD-NE2	6.61	126.31	116.40
1	D	401	GLN	CG-CD-NE2	6.60	126.29	116.40
1	B	51	HIS	CA-CB-CG	-6.49	107.31	113.80
1	B	401	GLN	CG-CD-NE2	6.33	125.89	116.40
1	D	438	GLU	N-CA-C	-6.23	100.76	110.42
1	A	72	ARG	N-CA-C	6.23	120.14	112.54
1	C	107	GLN	CG-CD-NE2	6.19	125.68	116.40
1	D	396	HIS	CA-CB-CG	6.16	119.96	113.80
1	B	52	PHE	N-CA-C	-6.07	104.23	111.69
1	A	52	PHE	N-CA-C	-6.05	104.97	112.90
1	D	142	VAL	N-CA-C	-6.05	104.41	111.00
1	A	191	PRO	CA-C-N	-5.94	115.20	123.10
1	A	191	PRO	C-N-CA	-5.94	115.20	123.10
1	D	135	GLU	N-CA-C	-5.83	96.93	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	HIS	CA-CB-CG	-5.75	108.05	113.80
1	B	403	HIS	CA-CB-CG	-5.75	108.05	113.80
1	D	134	ARG	N-CA-C	5.69	118.52	109.24
1	C	204	ARG	CA-C-N	-5.69	116.13	123.19
1	C	204	ARG	C-N-CA	-5.69	116.13	123.19
1	B	137	SER	N-CA-C	-5.64	98.80	110.80
1	C	364	GLY	N-CA-C	5.63	123.83	112.34
1	C	72	ARG	N-CA-C	5.53	119.29	112.54
1	B	205	VAL	CB-CA-C	5.49	118.57	110.77
1	C	212	SER	N-CA-C	5.45	117.85	109.07
1	A	313	SER	CA-C-N	5.27	127.91	122.80
1	A	313	SER	C-N-CA	5.27	127.91	122.80
1	D	339	LYS	CB-CA-C	5.24	118.67	111.23
1	C	177	LYS	N-CA-C	5.23	117.28	109.59
1	A	221	THR	CB-CA-C	5.15	118.95	109.99
1	D	306	VAL	N-CA-C	-5.09	104.25	108.63
1	C	51	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	150	LYS	N-CA-C	5.08	117.93	111.69
1	A	287	HIS	CA-CB-CG	5.05	118.85	113.80
1	D	339	LYS	N-CA-C	-5.00	97.78	107.44

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 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	3220	0	3206	86	0
1	B	3153	0	3154	90	0
1	C	3213	0	3194	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3305	0	3300	75	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	1	0
4	A	220	0	0	5	0
4	B	234	0	0	10	0
4	C	214	0	0	4	0
4	D	204	0	0	5	0
All	All	13779	0	12870	293	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 11.

All (293) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:117:SER:O	1:D:118:ALA:C	2.22	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:A:394:THR:C	1:A:395:VAL:HG22	2.07	0.77
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:HE2	1:A:363:LYS:HA	1.66	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:D:134:ARG:C	1:D:136:PRO:HD3	2.20	0.67
1:B:328:PHE:CE2	1:B:330:LEU:HD11	2.29	0.67
1:D:383:ASN:HD21	1:D:446:ARG:HH21	1.43	0.67
1:B:161:HIS:ND1	4:B:977:HOH:O	2.26	0.66
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: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:434:THR:O	1:B:435:THR:HB	1.96	0.64
1:B:239:LYS:NZ	1:B:460:ALA:HB1	2.12	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:467:HIS:O	1:D:468:HIS:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:41:GLU:CD	1:D:43:LEU:H	2.08	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:D:46:LEU:HD23	1:D:46:LEU:C	2.26	0.61
1:A:393:GLU:CD	1:B:175:ASN:HD22	2.08	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:D:440:MSE:HE1	1:D:444:LYS:C	2.27	0.59
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:A:132:GLN:O	1:A:133:ASP:CG	2.46	0.58
1:B:115:ARG:HA	1:B:154:LYS:HE2	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:332:GLU:HG2	1:D:342:GLN:HG2	1.85	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:C:65:LEU:O	1:C:72:ARG:HD3	2.04	0.57
1:D:162:GLY:O	1:D:166:HIS:HD2	1.88	0.57
1:D:89:TRP:HZ2	1:D:101:ALA:HB2	1.69	0.57
1:A:469:HIS:CD2	4:A:1065:HOH:O	2.57	0.57
1:C:329:GLN:HG3	4:C:1106:HOH:O	2.04	0.57
1:A:400:GLU:H	1:A:400:GLU:CD	2.13	0.57
1:D:336:ALA:C	1:D:337:ARG:HG2	2.29	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:A:398:SER:OG	1:A:400:GLU:OE1	2.17	0.56
1:D:362:GLY:HA3	1:D:418:THR:HG22	1.87	0.56
1:A:367:VAL:HG12	1:A:367:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:379:GLU:HG2	1:A:446:ARG:HD2	1.88	0.56
1:D:383:ASN:HD21	1:D:446:ARG:NH2	2.02	0.56
1:A:299:ARG:HH22	1:B:394:THR:HB	1.71	0.56
1:B:329:GLN:C	1:B:331:ALA:H	2.14	0.56
1:A:398:SER:HG	1:A:400:GLU:CD	2.14	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: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: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:C:95:PHE:O	1:C:465:HIS:HE1	1.91	0.54
1:D:164:LEU:HD22	1:D:285:LEU:HD13	1.89	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:46:LEU:C	1:C:46:LEU:HD23	2.33	0.53
1:B:271:LYS:NZ	4:B:1044:HOH:O	2.41	0.53
1:B:440:MSE:HE1	1:B:444:LYS:C	2.34	0.53
1:C:138:LYS:HD2	4:D:1068:HOH:O	2.08	0.53
1:C:434:THR:O	1:C:435:THR:CB	2.53	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: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:395:VAL:C	1:A:397:SER:H	2.17	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:329:GLN:C	1:B:331:ALA:N	2.69	0.51
1:D:132:GLN:C	1:D:134:ARG:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:NH1	1:C:408:GLU:OE1	2.43	0.51
1:D:176:ARG:HB2	1:D:299:ARG:HD2	1.92	0.51
1:C:110:GLY:HA3	1:C:152:SER:C	2.34	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:107:GLN:HG2	1:B:207:GLU:OE2	2.11	0.50
1:A:126:SER:O	1:A:129:GLU:OE1	2.29	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:A:138:LYS:CD	1:B:136:PRO:HG3	2.42	0.49
1:D:397:SER:OG	1:D:402:LEU:CD1	2.58	0.49
1:D:121:LEU:N	1:D:121:LEU:HD12	2.27	0.49
1:D:228:PHE:O	1:D:231:ARG:HG2	2.11	0.49
1:A:231:ARG:HA	1:A:231:ARG:NE	2.27	0.49
1:A:394:THR:C	1:A:395:VAL:HG13	2.37	0.49
1:A:144:PHE:HA	1:A:147:ASN:HD22	1.77	0.48
1:A:394:THR:O	1:A:395:VAL:CB	2.58	0.48
1:A:69:CYS:SG	1:A:204:ARG:HB3	2.53	0.48
1:A:46:LEU:C	1:A:46:LEU:HD23	2.38	0.48
1:A:113:GLN:HB2	1:A:114:PRO:HD3	1.95	0.48
1:B:46:LEU:C	1:B:46:LEU:HD23	2.39	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:C:465:HIS:HD2	1:D:382:GLU:OE2	1.97	0.48
1:C:467:HIS:CD2	1:C:468:HIS:N	2.81	0.48
1:A:398:SER:OG	1:A:400:GLU:CD	2.57	0.47
1:A:461:ALA:O	1:A:462:ALA:C	2.57	0.47
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:A:231:ARG:HA	1:A:231:ARG:HE	1.79	0.47
1:B:434:THR:O	1:B:435:THR:CB	2.61	0.47
1:C:90:SER:HA	1:C:94:VAL:HB	1.95	0.47
1:C:107:GLN:OE1	1:D:205:VAL:CG1	2.56	0.47
1:B:136:PRO:O	1:B:137:SER:CB	2.63	0.47
1:D:69:CYS:SG	1:D:204:ARG:HB3	2.55	0.47
1:B:317:ASP:OD2	3:B:6:GOL:H11	2.15	0.47
1:D:227:ASP:CG	1:D:231:ARG:HH21	2.23	0.47
1:A:143:ALA:O	1:A:147:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:OD1	1:A:308:CYS:SG	2.73	0.46
1:C:205:VAL:CG1	1:D:107:GLN:OE1	2.63	0.46
1:D:356:LYS:HG2	1:D:386:SER:OG	2.15	0.46
1:A:81:ARG:HH22	1:B:103:ASP:CG	2.24	0.46
1:B:136:PRO:HG2	1:B:137:SER:N	2.31	0.46
1:D:205:VAL:HG13	4:D:971:HOH:O	2.15	0.46
1:C:300:ASP:O	1:C:303:LYS:HE3	2.16	0.46
1:B:424:ASN:C	1:B:424:ASN:OD1	2.59	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: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:253:GLN:HA	1:C:258:ARG:O	2.16	0.45
1:B:357:VAL:HG21	1:B:449:LEU:HD13	1.97	0.45
1:C:419:GLU:O	1:C:422:LEU:HB2	2.17	0.45
1:D:317:ASP:OD2	3:D:5:GOL:O1	2.28	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:C:137:SER:HG	1:C:140:GLN:NE2	2.11	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: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: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:135:GLU:HG3	1:B:136:PRO:HD2	2.00	0.43
1:B:434:THR:HB	1:B:436:MSE:CE	2.46	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:A:115:ARG:O	1:A:116:ASP:C	2.61	0.43
1:B:402:LEU:HD12	1:B:402:LEU:HA	1.86	0.43
1:A:413:PHE:HB3	1:A:429:LEU:HD11	2.00	0.43
1:C:49:ARG:HH12	1:C:408:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:O	1:D:147:ASN:C	2.62	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
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:A:137:SER:O	1:A:141:LEU:HG	2.19	0.42
1:C:440:MSE:CE	1:C:445:LEU:HA	2.37	0.42
1:D:378:ASN:O	1:D:382:GLU:HG3	2.19	0.42
1:A:434:THR:O	1:A:435:THR:OG1	2.24	0.42
1:B:424:ASN:ND2	1:B:426:LEU:HG	2.34	0.42
1:D:190:HIS:HA	1:D:191:PRO:HD2	1.87	0.42
1:D:340:SER:O	1:D:341:LEU:C	2.62	0.42
1:A:399:LEU:HD23	1:A:437:LYS:NZ	2.34	0.42
1:B:383:ASN:ND2	1:B:446:ARG:HH21	1.97	0.42
1:A:137:SER:OG	1:A:138:LYS:N	2.51	0.42
1:B:44:VAL:HG11	1:B:60:LEU:HB3	2.02	0.42
1:C:161:HIS:O	1:C:165:GLU:HG3	2.19	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:148:LEU:HD23	1:D:148:LEU:HA	1.80	0.42
1:A:379:GLU:OE2	1:A:446:ARG:HD3	2.20	0.42
1:A:428:GLN:CD	1:A:437:LYS:HD3	2.45	0.42
1:B:282:ASP:C	1:B:282:ASP:OD1	2.62	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: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:B:208:LYS:HE3	1:B:315:ASP:CG	2.45	0.41
1:D:415:VAL:HG21	1:D:445:LEU:HD21	2.01	0.41
1:A:145:LEU:HD13	1:B:130:ILE:HG21	2.02	0.41
1:B:138:LYS:O	1:B:142:VAL:HB	2.20	0.41
1:B:399:LEU:HG	1:B:403:HIS:CE1	2.55	0.41
1:C:254:ASP:OD1	1:C:254:ASP:C	2.63	0.41
1:C:357:VAL:HG21	1:C:449:LEU:HD13	2.01	0.41
1:D:330:LEU:HD13	1:D:344:LYS:HG2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:112:SER:OG	1:C:150:LYS:HA	2.20	0.41
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.87	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: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:D:147:ASN:O	1:D:148:LEU:C	2.62	0.40
1:A:125:GLU:O	1:A:126:SER:C	2.64	0.40
1:A:360:ASP:CG	1:A:402:LEU:HD21	2.47	0.40
1:B:440:MSE:CE	1:B:444:LYS:C	2.94	0.40
1:C:363:LYS:CD	1:C:418:THR:HB	2.52	0.40
1:B:135:GLU:HA	1:B:136:PRO:HD2	1.92	0.40
1:B:190:HIS:HE1	1:B:208:LYS:CD	2.27	0.40
1:C:230:LEU:CD1	1:C:263:LEU:HD21	2.52	0.40
1:A:357:VAL:CG1	1:A:387:VAL:HG22	2.51	0.40
1:A:424:ASN:OD1	1:A:424:ASN:C	2.64	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:C:205:VAL:HG13	1:D:107:GLN:CD	2.34	0.40
1:D:69:CYS:SG	1:D:204:ARG:HG3	2.62	0.40
1:D:440:MSE:HE2	1:D:440:MSE:HB3	1.93	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%)	12 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	389/454 (86%)	378 (97%)	6 (2%)	5 (1%)	9	3
1	C	397/454 (87%)	385 (97%)	9 (2%)	3 (1%)	16	8
1	D	409/454 (90%)	387 (95%)	18 (4%)	4 (1%)	12	5
All	All	1592/1816 (88%)	1533 (96%)	43 (3%)	16 (1%)	12	5

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
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%)	345 (97%)	12 (3%)	32	23
1	B	349/391 (89%)	333 (95%)	16 (5%)	24	13
1	C	355/391 (91%)	337 (95%)	18 (5%)	21	10
1	D	365/391 (93%)	352 (96%)	13 (4%)	31	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1426/1564 (91%)	1367 (96%)	59 (4%)	27	17

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	129	GLU
1	A	191	PRO
1	A	205	VAL
1	A	221	THR
1	A	231	ARG
1	A	350	PRO
1	A	393	GLU
1	A	438	GLU
1	A	440	MSE
1	A	464	ASP
1	A	469	HIS
1	B	81	ARG
1	B	92	MSE
1	B	107	GLN
1	B	129	GLU
1	B	131	LEU
1	B	154	LYS
1	B	177	LYS
1	B	205	VAL
1	B	255	GLU
1	B	377	LEU
1	B	394	THR
1	B	402	LEU
1	B	431	SER
1	B	436	MSE
1	B	440	MSE
1	B	455	SER
1	C	49	ARG
1	C	82	LYS
1	C	92	MSE
1	C	96	ARG
1	C	117	SER
1	C	191	PRO
1	C	205	VAL
1	C	329	GLN
1	C	357	VAL

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Mol	Chain	Res	Type
1	C	392	SER
1	C	399	LEU
1	C	414	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	292	ASN
1	D	303	LYS
1	D	309	VAL
1	D	399	LEU
1	D	400	GLU
1	D	402	LEU
1	D	426	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	166	HIS
1	A	232	HIS
1	A	279	ASN
1	A	283	GLN
1	A	292	ASN
1	A	374	GLN
1	A	428	GLN
1	A	466	HIS
1	A	468	HIS
1	B	58	GLN
1	B	175	ASN
1	B	190	HIS
1	B	253	GLN
1	B	297	GLN
1	B	371	GLN

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Mol	Chain	Res	Type
1	B	383	ASN
1	B	403	HIS
1	B	428	GLN
1	C	140	GLN
1	C	166	HIS
1	C	283	GLN
1	C	292	ASN
1	C	329	GLN
1	C	465	HIS
1	C	468	HIS
1	D	58	GLN
1	D	98	GLN
1	D	107	GLN
1	D	166	HIS
1	D	232	HIS
1	D	292	ASN
1	D	383	ASN
1	D	468	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	5	-	5,5,5	0.50	0	5,5,5	0.32	0
3	GOL	B	6	-	5,5,5	0.38	0	5,5,5	0.85	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	D	5	-	-	2/4/4/4	-
3	GOL	B	6	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	6	GOL	O1-C1-C2-O2
3	B	6	GOL	O1-C1-C2-C3
3	B	6	GOL	C1-C2-C3-O3
3	D	5	GOL	C1-C2-C3-O3
3	B	6	GOL	O2-C2-C3-O3
3	D	5	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	GOL	1	0
3	B	6	GOL	1	0

5.7 Other polymers [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.