



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:43 am BST

PDB ID : 4MYH
Title : Structure of the Glutathione bound mitochondrial ABC transporter, Atm1
Authors : Srinivasan, V.
Deposited on : 2013-09-27
Resolution : 3.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

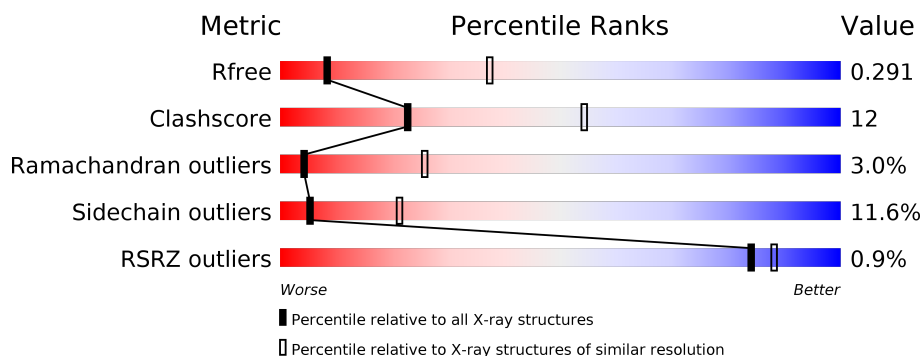
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	598	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>6%</div> </div> </div>
1	B	598	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>6%</div> </div> </div>
1	C	598	<div> <div></div> <div> <div></div> <div>73%</div> <div>22%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14048 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.

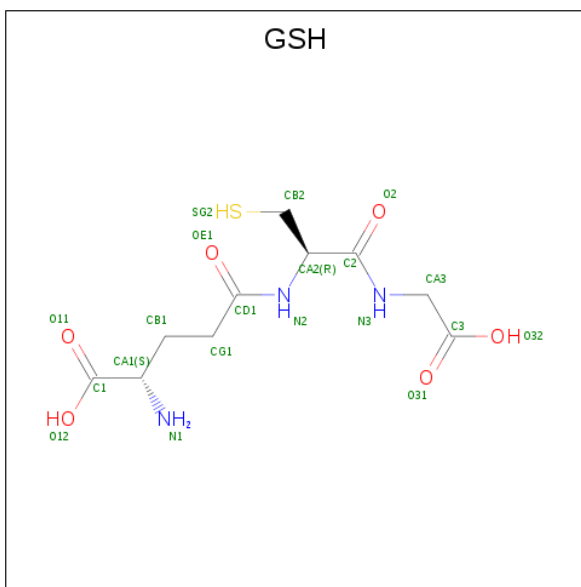
- Molecule 1 is a protein called Iron-sulfur clusters transporter ATM1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			
1	C	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			
1	B	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	TRP	-	EXPRESSION TAG	UNP P40416
A	692	SER	-	EXPRESSION TAG	UNP P40416
A	693	HIS	-	EXPRESSION TAG	UNP P40416
A	694	PRO	-	EXPRESSION TAG	UNP P40416
A	695	GLN	-	EXPRESSION TAG	UNP P40416
C	691	TRP	-	EXPRESSION TAG	UNP P40416
C	692	SER	-	EXPRESSION TAG	UNP P40416
C	693	HIS	-	EXPRESSION TAG	UNP P40416
C	694	PRO	-	EXPRESSION TAG	UNP P40416
C	695	GLN	-	EXPRESSION TAG	UNP P40416
B	691	TRP	-	EXPRESSION TAG	UNP P40416
B	692	SER	-	EXPRESSION TAG	UNP P40416
B	693	HIS	-	EXPRESSION TAG	UNP P40416
B	694	PRO	-	EXPRESSION TAG	UNP P40416
B	695	GLN	-	EXPRESSION TAG	UNP P40416

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).

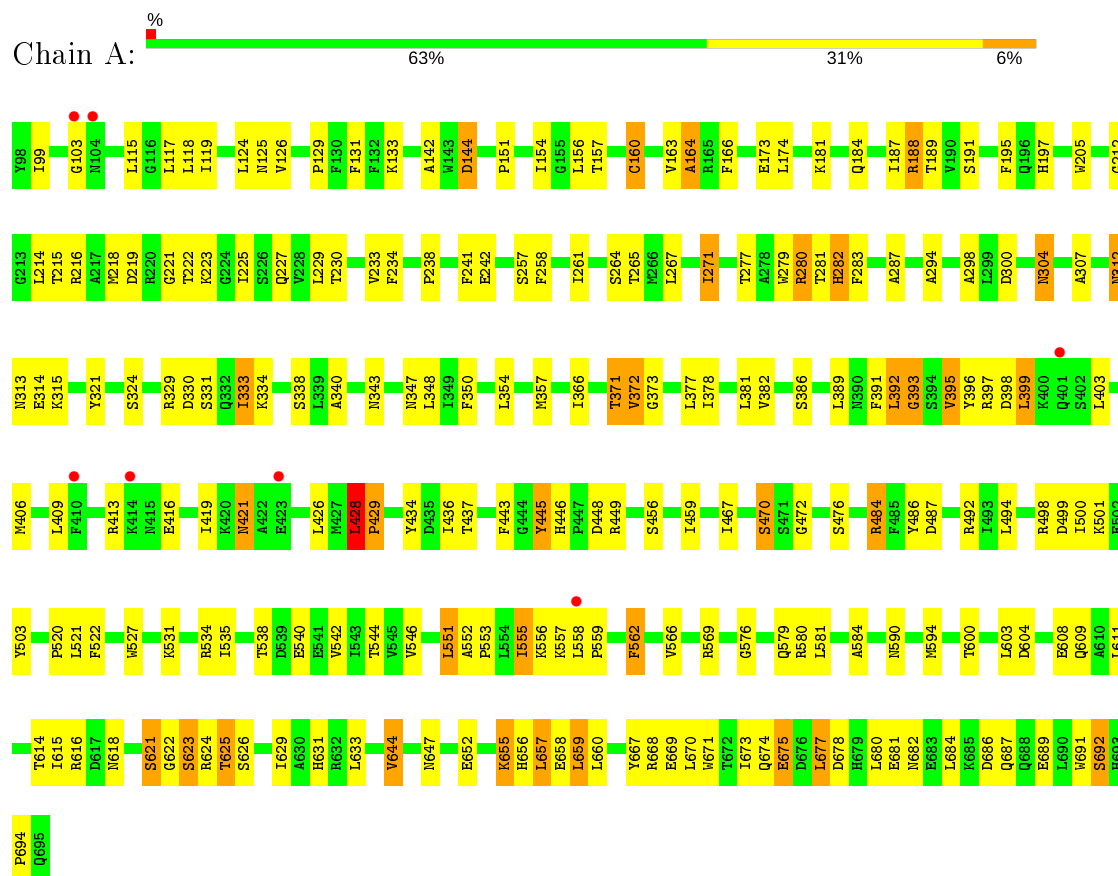


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

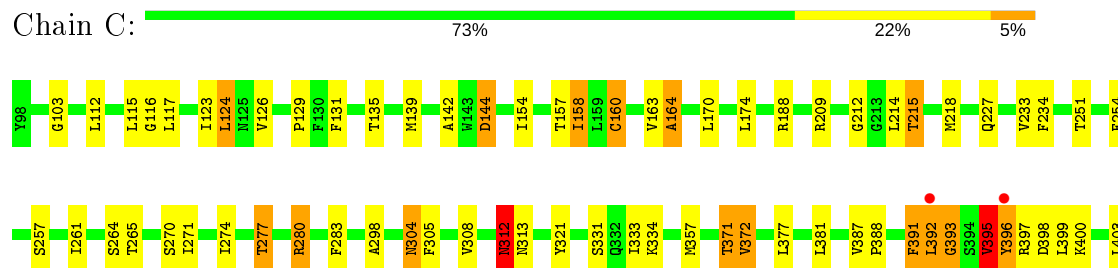
3 Residue-property plots

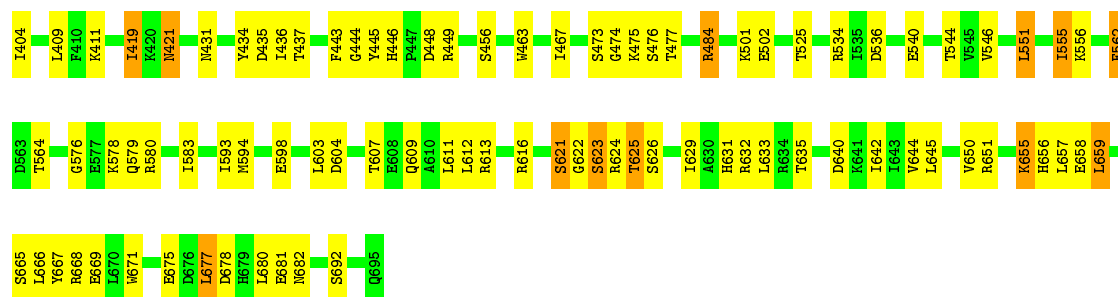
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Iron-sulfur clusters transporter ATM1, mitochondrial

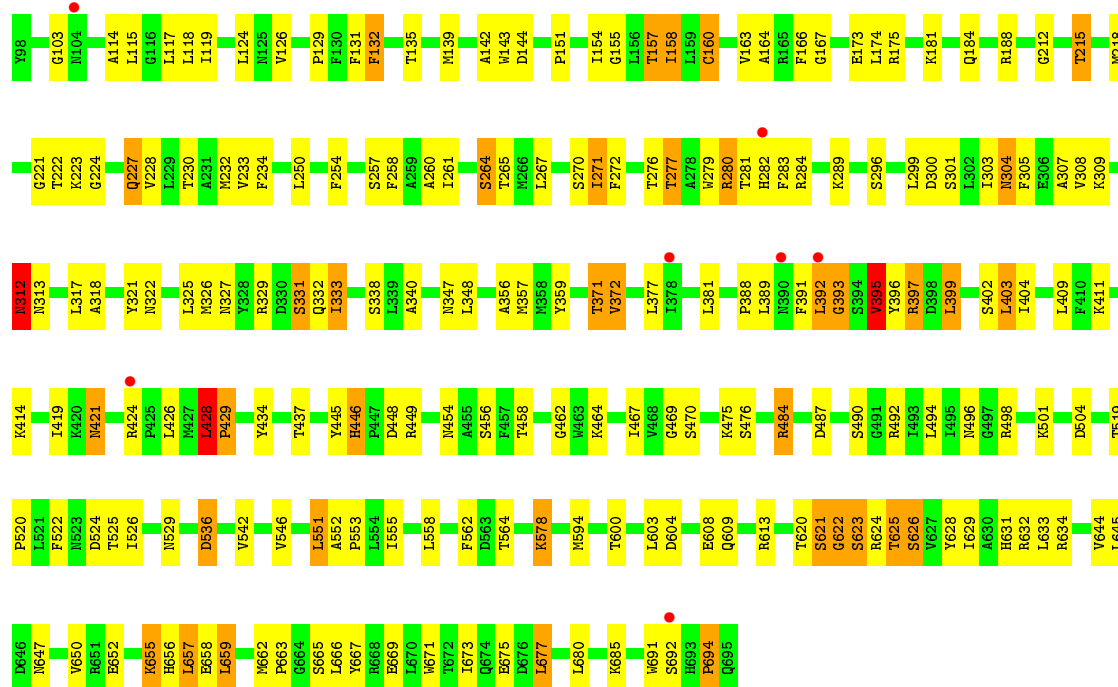


- Molecule 1: Iron-sulfur clusters transporter ATM1, mitochondrial





- Molecule 1: Iron-sulfur clusters transporter ATM1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.69Å 157.69Å 523.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.99 – 3.38 58.99 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.99-3.38) 99.6 (58.99-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.247 , 0.290 0.249 , 0.291	Depositor DCC
R_{free} test set	2782 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14048	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.59	0/4763	0.66	0/6451
1	B	0.56	0/4763	0.65	1/6451 (0.0%)
1	C	0.53	0/4763	0.64	0/6451
All	All	0.56	0/14289	0.65	1/19353 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	LEU	C-N-CD	-6.73	105.80	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	428	LEU	Peptide
1	B	428	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4676	0	4738	141	0
1	B	4676	0	4738	145	0
1	C	4676	0	4738	74	0
2	B	20	0	15	3	0
All	All	14048	0	14229	326	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 12.

All (326) 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:B:261:ILE:HD11	1:B:357:MET:HG3	1.59	0.84
1:A:531:LYS:NZ	1:A:535:ILE:O	2.12	0.82
1:A:443:PHE:HZ	1:A:486:TYR:HD1	1.31	0.78
1:A:472:GLY:HA3	1:B:694:PRO:HG3	1.64	0.77
1:A:280:ARG:NH1	1:A:338:SER:OG	2.18	0.77
1:A:218:MET:HA	1:A:409:LEU:HD13	1.67	0.76
1:C:261:ILE:HD11	1:C:357:MET:HG3	1.67	0.76
1:A:188:ARG:HD2	1:B:326:MET:HG3	1.68	0.76
1:A:484:ARG:NH1	1:A:501:LYS:HG2	2.01	0.75
1:B:280:ARG:NH2	2:B:701:GSH:SG2	2.58	0.74
1:C:218:MET:HA	1:C:409:LEU:HD13	1.70	0.74
1:B:280:ARG:NH1	1:B:338:SER:OG	2.18	0.73
1:B:391:PHE:O	1:B:393:GLY:N	2.22	0.72
1:A:283:PHE:HE1	1:A:334:LYS:HD3	1.55	0.71
1:A:350:PHE:CE1	1:A:386:SER:HB3	2.25	0.71
1:C:594:MET:HE1	1:C:624:ARG:HH21	1.56	0.71
1:A:197:HIS:CD2	1:A:413:ARG:HA	2.27	0.70
1:C:431:ASN:H	1:B:492:ARG:HH22	1.38	0.69
1:B:621:SER:O	1:B:623:SER:N	2.24	0.69
1:A:428:LEU:HB3	1:A:429:PRO:HD3	1.74	0.69
1:B:284:ARG:NH2	2:B:701:GSH:O2	2.26	0.68
1:B:546:VAL:HG13	1:B:551:LEU:HB3	1.74	0.68
1:A:520:PRO:HG3	1:B:307:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:MET:HE1	1:A:624:ARG:HH21	1.59	0.67
1:C:621:SER:O	1:C:623:SER:N	2.28	0.66
1:A:261:ILE:HD11	1:A:357:MET:HG3	1.75	0.66
1:C:397:ARG:NH1	1:C:398:ASP:OD1	2.28	0.66
1:A:391:PHE:O	1:A:393:GLY:N	2.30	0.65
1:A:421:ASN:OD1	1:A:421:ASN:N	2.30	0.64
1:C:546:VAL:HG13	1:C:551:LEU:HB3	1.79	0.64
1:A:173:GLU:HB3	1:B:340:ALA:HB1	1.79	0.64
1:A:669:GLU:O	1:A:673:ILE:HG13	1.98	0.64
1:C:651:ARG:HD3	1:C:666:LEU:HD22	1.79	0.64
1:B:652:GLU:OE2	1:B:666:LEU:N	2.24	0.64
1:A:546:VAL:HG13	1:A:551:LEU:HB3	1.80	0.63
1:B:218:MET:HA	1:B:409:LEU:HD13	1.80	0.63
1:B:632:ARG:HD2	1:B:634:ARG:NH2	2.13	0.63
1:B:594:MET:HE1	1:B:624:ARG:HH21	1.63	0.62
1:B:126:VAL:O	1:B:129:PRO:HD2	1.98	0.62
1:C:484:ARG:NH1	1:C:501:LYS:HG2	2.14	0.62
1:C:395:VAL:O	1:C:397:ARG:N	2.32	0.61
1:A:436:ILE:HB	1:A:459:ILE:HB	1.81	0.61
1:A:184:GLN:HB3	1:B:329:ARG:HG3	1.83	0.61
1:B:429:PRO:HD3	1:B:498:ARG:NH1	2.15	0.61
1:B:421:ASN:OD1	1:B:421:ASN:N	2.19	0.61
1:A:340:ALA:HB1	1:B:173:GLU:HB3	1.82	0.60
1:B:632:ARG:HD2	1:B:634:ARG:HH21	1.67	0.60
1:A:684:LEU:HA	1:B:680:LEU:HD23	1.84	0.60
1:A:484:ARG:NH1	1:A:487:ASP:OD2	2.34	0.60
1:C:656:HIS:HE1	1:C:671:TRP:CZ3	2.20	0.60
1:A:283:PHE:CE1	1:A:334:LYS:HD3	2.37	0.60
1:B:632:ARG:HH11	1:B:634:ARG:HH22	1.48	0.59
1:A:579:GLN:HB2	1:A:611:LEU:HD11	1.84	0.59
1:A:633:LEU:HD12	1:A:633:LEU:H	1.68	0.59
1:A:233:VAL:HG12	1:A:234:PHE:CD1	2.38	0.59
1:B:446:HIS:ND1	1:B:448:ASP:OD1	2.36	0.59
1:B:434:TYR:O	1:B:625:THR:HG21	2.03	0.58
1:A:133:LYS:HG3	1:A:373:GLY:HA3	1.85	0.58
1:A:633:LEU:HD23	1:A:667:TYR:CE1	2.39	0.58
1:B:118:LEU:HD13	1:B:175:ARG:HH11	1.67	0.58
1:A:670:LEU:O	1:A:674:GLN:HB2	2.03	0.58
1:A:313:ASN:O	1:A:315:LYS:N	2.37	0.57
1:B:250:LEU:HD13	1:B:258:PHE:HB3	1.85	0.57
1:B:377:LEU:O	1:B:381:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:GLU:O	1:C:544:THR:HG23	2.04	0.57
1:B:280:ARG:HH21	2:B:701:GSH:HSG	1.49	0.57
1:C:396:TYR:O	1:C:400:LYS:HG2	2.05	0.56
1:A:434:TYR:O	1:A:625:THR:HG21	2.06	0.56
1:A:197:HIS:CD2	1:A:413:ARG:HG2	2.41	0.55
1:B:645:LEU:HD23	1:B:650:VAL:HA	1.87	0.55
1:C:254:PHE:HZ	1:C:377:LEU:HD23	1.71	0.55
1:B:492:ARG:HD2	1:B:494:LEU:HD21	1.89	0.55
1:A:280:ARG:HH11	1:A:338:SER:HG	1.53	0.55
1:A:397:ARG:NH1	1:A:398:ASP:OD1	2.40	0.55
1:C:633:LEU:HD23	1:C:667:TYR:CE1	2.42	0.55
1:B:304:ASN:N	1:B:304:ASN:OD1	2.39	0.55
1:B:484:ARG:NH1	1:B:501:LYS:HG2	2.22	0.55
1:B:633:LEU:HD23	1:B:667:TYR:CE1	2.42	0.55
1:C:609:GLN:O	1:C:613:ARG:HG3	2.07	0.55
1:A:205:TRP:HH2	1:A:214:LEU:HD21	1.71	0.54
1:A:484:ARG:HH12	1:A:501:LYS:HG2	1.71	0.54
1:A:500:ILE:HA	1:A:503:TYR:HD2	1.72	0.54
1:A:377:LEU:O	1:A:381:LEU:HB2	2.08	0.54
1:C:209:ARG:HB3	1:C:214:LEU:HD11	1.88	0.54
1:B:600:THR:HB	1:B:608:GLU:HG3	1.89	0.54
1:A:181:LYS:HG3	1:B:333:ILE:HD11	1.90	0.54
1:B:395:VAL:O	1:B:397:ARG:N	2.41	0.54
1:A:540:GLU:O	1:A:544:THR:HG23	2.07	0.53
1:A:125:ASN:ND2	1:A:242:GLU:OE2	2.30	0.53
1:B:114:ALA:O	1:B:118:LEU:N	2.40	0.53
1:A:124:LEU:HD12	1:A:164:ALA:HA	1.91	0.53
1:A:678:ASP:O	1:A:682:ASN:HB2	2.08	0.53
1:A:590:ASN:O	1:A:590:ASN:ND2	2.41	0.52
1:C:502:GLU:OE2	1:B:424:ARG:HD3	2.09	0.52
1:B:484:ARG:NH1	1:B:487:ASP:OD2	2.42	0.52
1:B:469:GLY:O	1:B:475:LYS:NZ	2.40	0.52
1:B:154:ILE:HA	1:B:157:THR:HB	1.91	0.52
1:B:526:ILE:HD11	1:B:558:LEU:HD12	1.91	0.52
1:B:233:VAL:HG12	1:B:234:PHE:CD1	2.45	0.52
1:C:677:LEU:O	1:C:681:GLU:HG2	2.10	0.52
1:A:233:VAL:HG12	1:A:234:PHE:HD1	1.75	0.52
1:B:411:LYS:O	1:B:414:LYS:HB3	2.09	0.52
1:B:669:GLU:O	1:B:673:ILE:HG13	2.09	0.51
1:C:126:VAL:O	1:C:129:PRO:HD2	2.10	0.51
1:C:598:GLU:OE1	1:C:631:HIS:ND1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:ARG:HH11	1:B:634:ARG:NH2	2.08	0.51
1:A:527:TRP:HD1	1:A:562:PHE:CD2	2.29	0.51
1:C:304:ASN:O	1:C:308:VAL:HG13	2.11	0.51
1:C:434:TYR:O	1:C:625:THR:HG21	2.11	0.51
1:A:281:THR:C	1:A:283:PHE:H	2.13	0.51
1:A:500:ILE:HA	1:A:503:TYR:CD2	2.46	0.51
1:A:118:LEU:HD11	1:A:238:PRO:HG3	1.92	0.51
1:A:119:ILE:HG23	1:A:241:PHE:CE2	2.46	0.51
1:A:348:LEU:HB2	1:B:166:PHE:CE1	2.46	0.51
1:A:267:LEU:O	1:A:271:ILE:HG12	2.11	0.51
1:C:154:ILE:O	1:C:158:ILE:HG23	2.11	0.51
1:A:205:TRP:CH2	1:A:214:LEU:HD21	2.46	0.50
1:C:304:ASN:OD1	1:C:304:ASN:N	2.43	0.50
1:C:579:GLN:HB2	1:C:611:LEU:HD11	1.92	0.50
1:B:129:PRO:HB2	1:B:377:LEU:HD12	1.93	0.50
1:B:221:GLY:HA3	1:B:409:LEU:HD22	1.93	0.50
1:A:133:LYS:HE3	1:A:371:THR:HG21	1.93	0.50
1:A:443:PHE:CZ	1:A:486:TYR:HD1	2.19	0.50
1:A:527:TRP:HB2	1:A:562:PHE:HB3	1.94	0.50
1:A:691:TRP:CH2	1:B:631:HIS:HB2	2.47	0.50
1:A:329:ARG:NH2	1:A:330:ASP:OD1	2.43	0.49
1:A:522:PHE:CD1	1:B:300:ASP:HB3	2.46	0.49
1:B:426:LEU:HB3	1:B:428:LEU:HD23	1.94	0.49
1:A:426:LEU:HB3	1:A:428:LEU:HG	1.94	0.49
1:A:428:LEU:HB2	1:A:503:TYR:HE1	1.77	0.49
1:A:197:HIS:HD2	1:A:413:ARG:HG2	1.78	0.49
1:C:436:ILE:HD11	1:C:593:ILE:HD13	1.93	0.49
1:B:131:PHE:CD2	1:B:160:CYS:HB3	2.48	0.49
1:B:524:ASP:OD1	1:B:525:THR:N	2.44	0.49
1:B:655:LYS:O	1:B:659:LEU:HB2	2.13	0.49
1:A:600:THR:HB	1:A:608:GLU:HG3	1.94	0.48
1:B:139:MET:SD	1:B:154:ILE:HD12	2.53	0.48
1:C:678:ASP:O	1:C:682:ASN:HB2	2.13	0.48
1:A:521:LEU:HD13	1:A:566:VAL:HB	1.95	0.48
1:A:184:GLN:HG3	1:B:332:GLN:HB3	1.95	0.48
1:C:129:PRO:HG2	1:C:381:LEU:HD12	1.94	0.48
1:A:191:SER:O	1:B:321:TYR:HE2	1.95	0.48
1:A:644:VAL:HG13	1:A:652:GLU:HB2	1.96	0.48
1:C:656:HIS:CE1	1:C:671:TRP:CZ3	3.01	0.48
1:A:445:TYR:CE1	1:A:486:TYR:HE1	2.31	0.48
1:A:307:ALA:HB2	1:B:520:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:HA	1:B:173:GLU:OE1	2.14	0.48
1:C:645:LEU:HD23	1:C:650:VAL:HA	1.95	0.48
1:A:131:PHE:CD2	1:A:160:CYS:HB3	2.49	0.48
1:A:258:PHE:HE1	1:A:378:ILE:HD12	1.78	0.48
1:C:421:ASN:OD1	1:C:421:ASN:N	2.42	0.48
1:C:555:ILE:HG21	1:C:562:PHE:CE1	2.49	0.48
1:A:686:ASP:O	1:A:689:GLU:HB3	2.13	0.48
1:A:492:ARG:HD2	1:A:494:LEU:HD21	1.96	0.48
1:B:277:THR:HA	1:B:280:ARG:HG2	1.95	0.48
1:A:126:VAL:O	1:A:129:PRO:HD2	2.13	0.47
1:B:254:PHE:HB3	1:B:258:PHE:CD2	2.49	0.47
1:A:221:GLY:HA3	1:A:409:LEU:HD22	1.96	0.47
1:A:687:GLN:HB3	1:B:677:LEU:HD12	1.96	0.47
1:B:218:MET:O	1:B:222:THR:HG23	2.15	0.47
1:A:279:TRP:O	1:A:282:HIS:ND1	2.47	0.47
1:B:421:ASN:ND2	1:B:504:ASP:OD1	2.47	0.47
1:A:212:GLY:O	1:A:216:ARG:HG3	2.14	0.47
1:A:333:ILE:HD11	1:B:181:LYS:HA	1.97	0.47
1:B:519:THR:O	1:B:578:LYS:NZ	2.48	0.47
1:A:689:GLU:HA	1:A:692:SER:HB3	1.97	0.47
1:B:685:LYS:HE2	1:B:685:LYS:HB3	1.75	0.47
1:B:254:PHE:CZ	1:B:377:LEU:HD23	2.50	0.47
1:B:462:GLY:H	1:B:625:THR:HB	1.79	0.47
1:C:371:THR:OG1	1:C:372:VAL:N	2.48	0.47
1:A:283:PHE:O	1:A:287:ALA:N	2.48	0.47
1:A:428:LEU:HB3	1:A:429:PRO:CD	2.42	0.47
1:C:112:LEU:O	1:C:116:GLY:N	2.42	0.47
1:A:294:ALA:HB2	1:A:324:SER:HB3	1.97	0.47
1:A:195:PHE:CE2	1:B:318:ALA:HA	2.49	0.47
1:B:536:ASP:OD2	1:B:536:ASP:N	2.36	0.47
1:A:558:LEU:HA	1:A:559:PRO:HD2	1.78	0.46
1:B:322:ASN:HA	1:B:325:LEU:HB2	1.97	0.46
1:A:283:PHE:CE1	1:A:334:LYS:HB3	2.50	0.46
1:A:304:ASN:N	1:A:304:ASN:OD1	2.47	0.46
1:B:496:ASN:O	1:B:498:ARG:HD2	2.15	0.46
1:C:633:LEU:HD12	1:C:633:LEU:H	1.80	0.46
1:B:633:LEU:HD12	1:B:633:LEU:H	1.80	0.46
1:C:270:SER:O	1:C:274:ILE:HG13	2.15	0.46
1:A:129:PRO:HB2	1:A:377:LEU:HD12	1.97	0.46
1:A:181:LYS:HA	1:B:333:ILE:HD11	1.97	0.46
1:B:542:VAL:O	1:B:546:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD13	1:C:174:LEU:HB3	1.97	0.46
1:C:473:SER:OG	1:C:475:LYS:HG2	2.16	0.46
1:A:655:LYS:O	1:A:659:LEU:HB2	2.15	0.46
1:A:656:HIS:HE1	1:A:671:TRP:CZ3	2.34	0.46
1:B:558:LEU:HD13	1:B:564:THR:HG21	1.98	0.46
1:C:391:PHE:O	1:C:393:GLY:N	2.49	0.46
1:A:416:GLU:HG2	1:A:416:GLU:H	1.61	0.46
1:A:429:PRO:HB2	1:A:434:TYR:HE1	1.79	0.46
1:B:212:GLY:O	1:B:215:THR:HG22	2.16	0.46
1:C:397:ARG:HG3	1:C:398:ASP:H	1.81	0.46
1:A:581:LEU:O	1:A:584:ALA:HB3	2.16	0.46
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.99	0.45
1:C:594:MET:CE	1:C:624:ARG:HH21	2.25	0.45
1:B:620:THR:O	1:B:622:GLY:N	2.49	0.45
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.80	0.45
1:A:329:ARG:HG3	1:B:184:GLN:HB3	1.96	0.45
1:B:280:ARG:HH11	1:B:338:SER:HG	1.55	0.45
1:B:299:LEU:O	1:B:303:ILE:HG13	2.16	0.45
1:B:428:LEU:HB3	1:B:429:PRO:HD3	1.99	0.45
1:A:225:ILE:HG12	1:A:406:MET:HG3	1.98	0.45
1:B:254:PHE:HZ	1:B:377:LEU:HD23	1.81	0.45
1:B:421:ASN:HD22	1:B:504:ASP:HA	1.82	0.45
1:C:283:PHE:CD1	1:C:334:LYS:HB3	2.52	0.45
1:B:228:VAL:O	1:B:232:MET:HG2	2.16	0.45
1:B:371:THR:OG1	1:B:372:VAL:N	2.49	0.45
1:C:209:ARG:HH22	1:C:411:LYS:NZ	2.14	0.45
1:A:166:PHE:CE1	1:B:348:LEU:HB2	2.52	0.44
1:A:144:ASP:OD2	1:A:144:ASP:N	2.47	0.44
1:A:283:PHE:CD1	1:A:334:LYS:HB3	2.52	0.44
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.98	0.44
1:A:576:GLY:O	1:A:580:ARG:HB2	2.17	0.44
1:A:298:ALA:HB2	1:A:321:TYR:CE1	2.51	0.44
1:C:668:ARG:NH2	1:C:669:GLU:OE2	2.50	0.44
1:A:354:LEU:HD21	1:A:382:VAL:HG12	1.98	0.44
1:C:131:PHE:CD2	1:C:160:CYS:HB3	2.53	0.44
1:B:429:PRO:HB2	1:B:434:TYR:HE1	1.82	0.44
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.87	0.44
1:A:691:TRP:CZ2	1:B:470:SER:HA	2.53	0.44
1:B:526:ILE:O	1:B:529:ASN:N	2.51	0.44
1:A:527:TRP:CZ3	1:A:531:LYS:HD2	2.52	0.44
1:A:611:LEU:O	1:A:615:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:O	1:B:264:SER:HB2	2.18	0.44
1:A:470:SER:HA	1:B:691:TRP:CZ2	2.53	0.44
1:A:371:THR:OG1	1:A:372:VAL:N	2.50	0.43
1:B:280:ARG:HB2	1:B:338:SER:OG	2.19	0.43
1:B:662:MET:HA	1:B:663:PRO:HD2	1.89	0.43
1:B:281:THR:C	1:B:283:PHE:H	2.21	0.43
1:A:569:ARG:HH21	1:B:296:SER:HB2	1.83	0.43
1:A:219:ASP:OD1	1:A:223:LYS:HE3	2.19	0.43
1:A:173:GLU:OE1	1:B:340:ALA:HA	2.19	0.43
1:C:400:LYS:HA	1:C:400:LYS:HD3	1.83	0.43
1:A:343:ASN:HB2	1:B:173:GLU:OE1	2.18	0.43
1:B:464:LYS:HE3	1:B:628:TYR:CD2	2.53	0.43
1:C:642:ILE:HG21	1:C:667:TYR:HE1	1.83	0.43
1:A:555:ILE:HD11	1:A:556:LYS:NZ	2.33	0.43
1:A:366:ILE:HG12	1:B:143:TRP:CE3	2.53	0.43
1:C:576:GLY:O	1:C:580:ARG:HB2	2.19	0.43
1:B:224:GLY:HA2	1:B:402:SER:HB3	2.01	0.43
1:B:609:GLN:O	1:B:613:ARG:HG3	2.19	0.43
1:C:312:ASN:HB2	1:C:313:ASN:H	1.65	0.43
1:C:680:LEU:HD12	1:C:680:LEU:HA	1.87	0.43
1:A:166:PHE:HA	1:B:347:ASN:OD1	2.18	0.43
1:A:119:ILE:HG23	1:A:241:PHE:CZ	2.54	0.42
1:A:389:LEU:HA	1:A:389:LEU:HD12	1.86	0.42
1:B:305:PHE:O	1:B:308:VAL:HG22	2.18	0.42
1:B:327:ASN:O	1:B:331:SER:HB2	2.18	0.42
1:B:403:LEU:HA	1:B:403:LEU:HD22	1.76	0.42
1:A:187:ILE:HG12	1:A:222:THR:HB	2.02	0.42
1:A:445:TYR:CD1	1:A:486:TYR:HE1	2.37	0.42
1:A:657:LEU:HD12	1:A:657:LEU:HA	1.79	0.42
1:A:677:LEU:O	1:A:681:GLU:HG2	2.19	0.42
1:B:522:PHE:HB2	1:B:529:ASN:OD1	2.20	0.42
1:C:435:ASP:OD1	1:B:498:ARG:NH2	2.45	0.42
1:C:556:LYS:HA	1:C:556:LYS:HD3	1.84	0.42
1:C:633:LEU:HD23	1:C:667:TYR:CZ	2.55	0.42
1:A:151:PRO:O	1:A:154:ILE:HG12	2.19	0.42
1:A:671:TRP:O	1:A:675:GLU:HB2	2.19	0.42
1:C:144:ASP:N	1:C:144:ASP:OD2	2.53	0.42
1:C:212:GLY:O	1:C:215:THR:HG22	2.19	0.42
1:A:614:THR:O	1:A:618:ASN:ND2	2.44	0.42
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.86	0.42
1:A:448:ASP:OD1	1:A:449:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:HIS:HD2	1:A:657:LEU:HD13	1.85	0.42
1:C:443:PHE:CG	1:C:444:GLY:N	2.87	0.42
1:B:261:ILE:HD11	1:B:357:MET:CG	2.41	0.42
1:C:277:THR:HA	1:C:280:ARG:HG2	2.00	0.42
1:B:151:PRO:O	1:B:154:ILE:HG12	2.20	0.42
1:B:155:GLY:O	1:B:158:ILE:HG12	2.20	0.42
1:B:276:THR:O	1:B:279:TRP:HB3	2.20	0.42
1:B:356:ALA:O	1:B:359:TYR:HB3	2.19	0.42
1:B:594:MET:CE	1:B:624:ARG:HH21	2.32	0.42
1:A:538:THR:O	1:A:542:VAL:HG23	2.20	0.41
1:C:298:ALA:HB2	1:C:321:TYR:CE1	2.55	0.41
1:C:525:THR:HA	1:C:564:THR:O	2.20	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.94	0.41
1:B:254:PHE:HB3	1:B:258:PHE:CE2	2.54	0.41
1:B:312:ASN:HB2	1:B:313:ASN:H	1.64	0.41
1:A:631:HIS:HB2	1:B:691:TRP:CZ2	2.56	0.41
1:C:579:GLN:O	1:C:583:ILE:HG13	2.19	0.41
1:C:612:LEU:HD21	1:C:635:THR:HB	2.02	0.41
1:A:188:ARG:NH1	1:A:189:THR:OG1	2.48	0.41
1:B:117:LEU:HD13	1:B:174:LEU:HB3	2.02	0.41
1:B:656:HIS:HD2	1:B:657:LEU:HD13	1.84	0.41
1:C:419:ILE:H	1:C:419:ILE:HG13	1.59	0.41
1:B:258:PHE:HD1	1:B:357:MET:HG2	1.84	0.41
1:A:621:SER:O	1:A:623:SER:N	2.45	0.41
1:B:223:LYS:O	1:B:227:GLN:HB2	2.21	0.41
1:B:448:ASP:OD1	1:B:449:ARG:N	2.54	0.41
1:C:124:LEU:HD13	1:C:164:ALA:HA	2.01	0.41
1:B:267:LEU:O	1:B:271:ILE:HG12	2.21	0.41
1:B:389:LEU:HA	1:B:389:LEU:HD12	1.86	0.41
1:B:304:ASN:O	1:B:308:VAL:HG13	2.20	0.41
1:B:301:SER:OG	1:B:317:LEU:HD13	2.19	0.41
1:C:135:THR:O	1:C:139:MET:HG2	2.20	0.41
1:C:305:PHE:O	1:C:308:VAL:HG22	2.20	0.41
1:B:132:PHE:O	1:B:135:THR:HG22	2.21	0.41
1:C:387:VAL:HB	1:C:388:PRO:HD3	2.03	0.41
1:C:448:ASP:CG	1:C:449:ARG:HG3	2.41	0.41
1:B:270:SER:C	1:B:272:PHE:H	2.23	0.41
1:C:631:HIS:CE1	1:C:632:ARG:HG3	2.56	0.41
1:C:655:LYS:O	1:C:659:LEU:HB2	2.21	0.41
1:A:494:LEU:HD23	1:A:499:ASP:HA	2.03	0.41
1:B:475:LYS:HG3	1:B:476:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:OD1	1:B:166:PHE:HA	2.20	0.41
1:B:428:LEU:HB3	1:B:498:ARG:HH12	1.86	0.41
1:B:656:HIS:HE1	1:B:671:TRP:CZ3	2.39	0.41
1:C:377:LEU:O	1:C:381:LEU:HB2	2.21	0.41
1:B:124:LEU:HD13	1:B:167:GLY:HA3	2.03	0.40
1:C:474:GLY:C	1:C:476:SER:N	2.74	0.40
1:C:463:TRP:HB3	1:C:640:ASP:HB2	2.02	0.40
1:A:300:ASP:HB3	1:B:522:PHE:CE1	2.56	0.40
1:B:626:SER:HB2	1:B:628:TYR:HE2	1.86	0.40
1:A:660:LEU:HD23	1:A:668:ARG:HG2	2.03	0.40
1:B:309:LYS:HD3	1:B:309:LYS:HA	1.89	0.40
1:B:526:ILE:HD11	1:B:558:LEU:CD1	2.51	0.40
1:A:117:LEU:HD13	1:A:174:LEU:HB3	2.03	0.40
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.80	0.40
1:B:608:GLU:OE1	1:B:632:ARG:NH1	2.55	0.40
1:C:233:VAL:HG12	1:C:234:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/598 (100%)	541 (91%)	34 (6%)	21 (4%)	3	23
1	B	596/598 (100%)	540 (91%)	38 (6%)	18 (3%)	4	26
1	C	596/598 (100%)	542 (91%)	40 (7%)	14 (2%)	6	31
All	All	1788/1794 (100%)	1623 (91%)	112 (6%)	53 (3%)	4	26

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	392	LEU
1	A	395	VAL
1	A	621	SER
1	C	312	ASN
1	C	392	LEU
1	C	395	VAL
1	C	396	TYR
1	C	621	SER
1	B	312	ASN
1	B	392	LEU
1	B	395	VAL
1	B	396	TYR
1	B	429	PRO
1	B	621	SER
1	A	396	TYR
1	A	622	GLY
1	C	164	ALA
1	C	622	GLY
1	B	622	GLY
1	A	164	ALA
1	A	282	HIS
1	C	103	GLY
1	C	142	ALA
1	B	142	ALA
1	B	164	ALA
1	B	282	HIS
1	A	99	ILE
1	A	142	ALA
1	A	393	GLY
1	A	429	PRO
1	A	446	HIS
1	A	603	LEU
1	C	446	HIS
1	C	603	LEU
1	B	393	GLY
1	B	446	HIS
1	B	603	LEU
1	A	271	ILE
1	A	470	SER
1	A	694	PRO
1	B	271	ILE
1	B	428	LEU

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Mol	Chain	Res	Type
1	A	314	GLU
1	C	163	VAL
1	C	393	GLY
1	A	103	GLY
1	B	163	VAL
1	C	271	ILE
1	A	428	LEU
1	A	163	VAL
1	B	103	GLY
1	B	694	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/514 (98%)	446 (89%)	55 (11%)	6	24
1	B	501/514 (98%)	441 (88%)	60 (12%)	5	20
1	C	501/514 (98%)	442 (88%)	59 (12%)	5	20
All	All	1503/1542 (98%)	1329 (88%)	174 (12%)	5	21

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	144	ASP
1	A	156	LEU
1	A	157	THR
1	A	160	CYS
1	A	188	ARG
1	A	215	THR
1	A	227	GLN
1	A	230	THR
1	A	257	SER
1	A	264	SER
1	A	265	THR

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Mol	Chain	Res	Type
1	A	277	THR
1	A	280	ARG
1	A	304	ASN
1	A	312	ASN
1	A	331	SER
1	A	333	ILE
1	A	371	THR
1	A	372	VAL
1	A	392	LEU
1	A	395	VAL
1	A	399	LEU
1	A	403	LEU
1	A	419	ILE
1	A	421	ASN
1	A	428	LEU
1	A	437	THR
1	A	445	TYR
1	A	456	SER
1	A	467	ILE
1	A	476	SER
1	A	484	ARG
1	A	498	ARG
1	A	534	ARG
1	A	551	LEU
1	A	555	ILE
1	A	557	LYS
1	A	562	PHE
1	A	604	ASP
1	A	609	GLN
1	A	616	ARG
1	A	623	SER
1	A	625	THR
1	A	626	SER
1	A	629	ILE
1	A	644	VAL
1	A	647	ASN
1	A	655	LYS
1	A	657	LEU
1	A	658	GLU
1	A	659	LEU
1	A	675	GLU
1	A	677	LEU

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Mol	Chain	Res	Type
1	A	692	SER
1	C	115	LEU
1	C	123	ILE
1	C	124	LEU
1	C	144	ASP
1	C	157	THR
1	C	158	ILE
1	C	160	CYS
1	C	170	LEU
1	C	188	ARG
1	C	215	THR
1	C	227	GLN
1	C	251	THR
1	C	257	SER
1	C	264	SER
1	C	265	THR
1	C	277	THR
1	C	280	ARG
1	C	304	ASN
1	C	312	ASN
1	C	331	SER
1	C	333	ILE
1	C	371	THR
1	C	372	VAL
1	C	391	PHE
1	C	392	LEU
1	C	395	VAL
1	C	399	LEU
1	C	403	LEU
1	C	404	ILE
1	C	419	ILE
1	C	421	ASN
1	C	437	THR
1	C	445	TYR
1	C	456	SER
1	C	467	ILE
1	C	477	THR
1	C	484	ARG
1	C	534	ARG
1	C	536	ASP
1	C	551	LEU
1	C	555	ILE

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Mol	Chain	Res	Type
1	C	562	PHE
1	C	578	LYS
1	C	604	ASP
1	C	607	THR
1	C	616	ARG
1	C	623	SER
1	C	625	THR
1	C	626	SER
1	C	629	ILE
1	C	644	VAL
1	C	655	LYS
1	C	657	LEU
1	C	658	GLU
1	C	659	LEU
1	C	665	SER
1	C	675	GLU
1	C	677	LEU
1	C	692	SER
1	B	115	LEU
1	B	119	ILE
1	B	132	PHE
1	B	144	ASP
1	B	157	THR
1	B	158	ILE
1	B	160	CYS
1	B	188	ARG
1	B	215	THR
1	B	227	GLN
1	B	230	THR
1	B	257	SER
1	B	264	SER
1	B	265	THR
1	B	277	THR
1	B	280	ARG
1	B	289	LYS
1	B	304	ASN
1	B	312	ASN
1	B	331	SER
1	B	333	ILE
1	B	371	THR
1	B	372	VAL
1	B	388	PRO

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Mol	Chain	Res	Type
1	B	392	LEU
1	B	395	VAL
1	B	397	ARG
1	B	399	LEU
1	B	403	LEU
1	B	404	ILE
1	B	419	ILE
1	B	421	ASN
1	B	437	THR
1	B	445	TYR
1	B	454	ASN
1	B	456	SER
1	B	458	THR
1	B	467	ILE
1	B	484	ARG
1	B	490	SER
1	B	536	ASP
1	B	551	LEU
1	B	555	ILE
1	B	562	PHE
1	B	578	LYS
1	B	604	ASP
1	B	623	SER
1	B	625	THR
1	B	626	SER
1	B	629	ILE
1	B	644	VAL
1	B	647	ASN
1	B	655	LYS
1	B	657	LEU
1	B	658	GLU
1	B	659	LEU
1	B	665	SER
1	B	675	GLU
1	B	677	LEU
1	B	692	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	379	ASN

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Mol	Chain	Res	Type
1	A	380	GLN
1	A	647	ASN
1	B	379	ASN
1	B	384	GLN
1	B	415	ASN
1	B	695	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GSH	B	701	-	12,19,19	2.47	3 (25%)	15,24,24	2.04	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	B	701	-	-	7/18/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GSH	CD1-N2	5.61	1.46	1.34
2	B	701	GSH	C2-N3	5.53	1.45	1.33
2	B	701	GSH	CB2-SG2	-2.48	1.76	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GSH	CA2-CB2-SG2	-5.66	107.83	114.19
2	B	701	GSH	CB2-CA2-C2	2.70	115.34	109.76
2	B	701	GSH	CB1-CG1-CD1	-2.65	107.12	113.04
2	B	701	GSH	C2-CA2-N2	2.18	117.09	111.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	GSH	N1-CA1-CB1-CG1
2	B	701	GSH	C1-CA1-CB1-CG1
2	B	701	GSH	N2-CA2-CB2-SG2
2	B	701	GSH	C2-CA2-CB2-SG2
2	B	701	GSH	OE1-CD1-CG1-CB1
2	B	701	GSH	N2-CD1-CG1-CB1
2	B	701	GSH	CA1-CB1-CG1-CD1

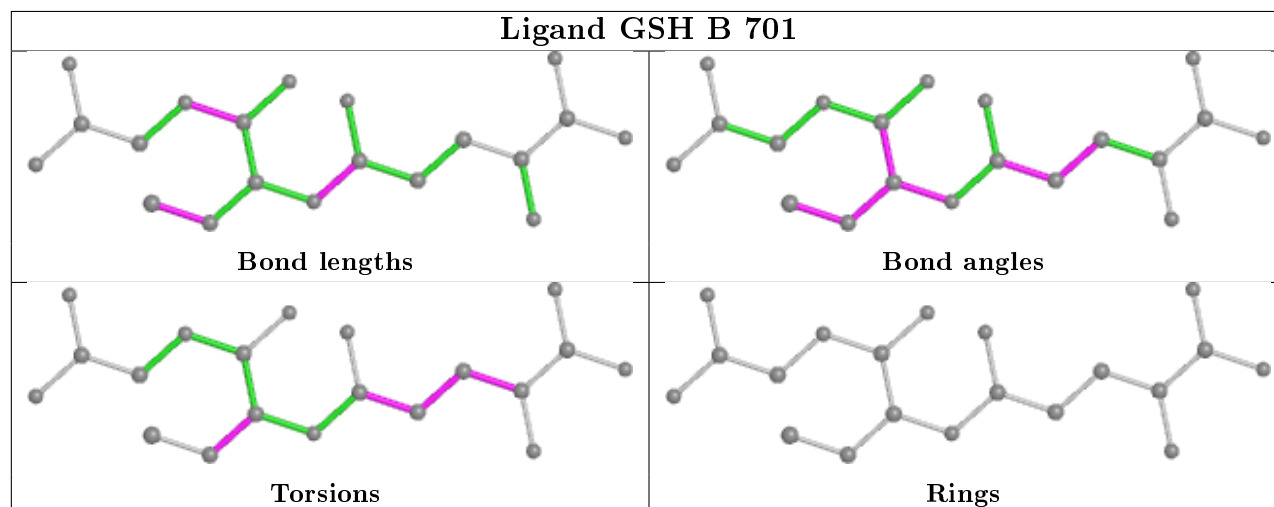
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	GSH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	598/598 (100%)	0.08	7 (1%) 79 83	12, 41, 59, 82	0
1	B	598/598 (100%)	-0.00	7 (1%) 79 83	9, 37, 53, 70	0
1	C	598/598 (100%)	-0.03	2 (0%) 94 96	8, 28, 46, 63	0
All	All	1794/1794 (100%)	0.01	16 (0%) 84 88	8, 35, 55, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	ASN	5.4
1	B	282	HIS	3.8
1	A	401	GLN	3.4
1	C	392	LEU	2.6
1	B	692	SER	2.5
1	A	423	GLU	2.4
1	B	392	LEU	2.4
1	A	103	GLY	2.4
1	C	396	TYR	2.4
1	A	414	LYS	2.2
1	B	424	ARG	2.2
1	A	558	LEU	2.1
1	A	410	PHE	2.1
1	B	378	ILE	2.1
1	B	104	ASN	2.0
1	B	390	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

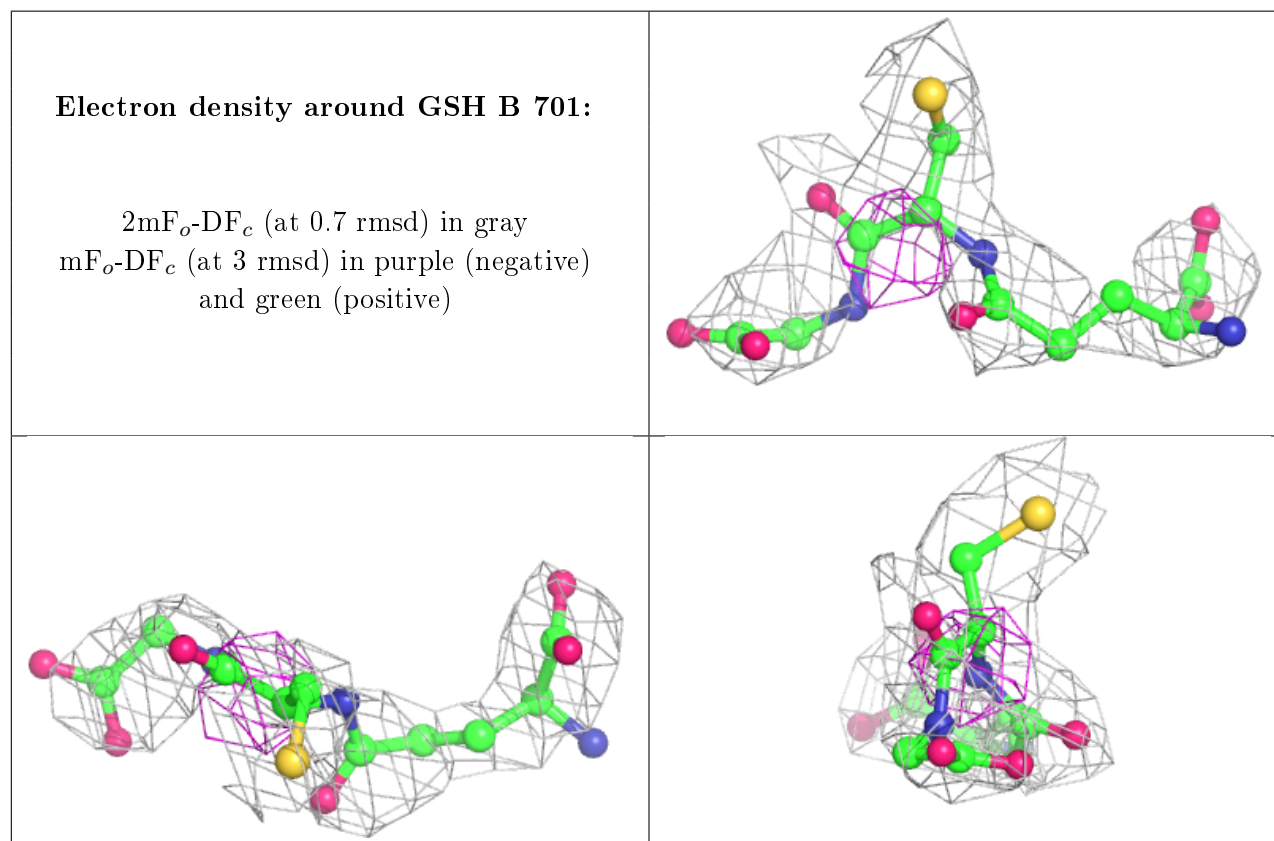
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GSH	B	701	20/20	0.81	0.40	61,66,71,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.