



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1G5I
Title : CRYSTAL STRUCTURE OF THE ACCESSORY SUBUNIT OF MURINE
MITOCHONDRIAL POLYMERASE GAMMA
Authors : Carrodegua, J.A.; Theis, K.; Bogenhagen, D.F.; Kisker, C.
Deposited on : 2000-11-01
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

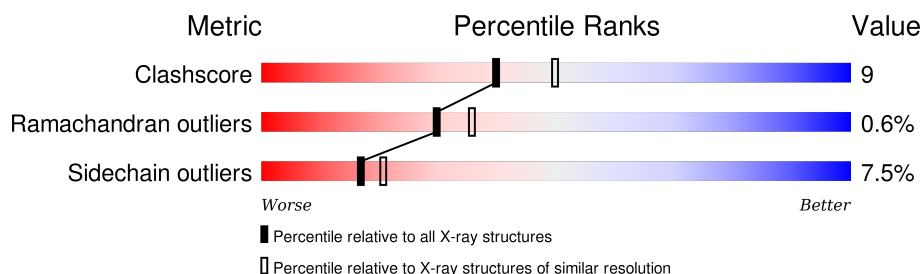
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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. 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.

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 13774 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	0	0	0
			3216	2050	570	582	14			
1	B	397	Total	C	N	O	S	0	0	0
			3149	2010	554	571	14			
1	C	405	Total	C	N	O	S	0	0	0
			3209	2045	568	582	14			
1	D	415	Total	C	N	O	S	0	0	0
			3302	2103	587	598	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	469	HIS	-	EXPRESSION TAG	UNP Q9QZM2
B	470	HIS	-	EXPRESSION TAG	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	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
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: C₃H₈O₃).



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

- Molecule 4 is water.

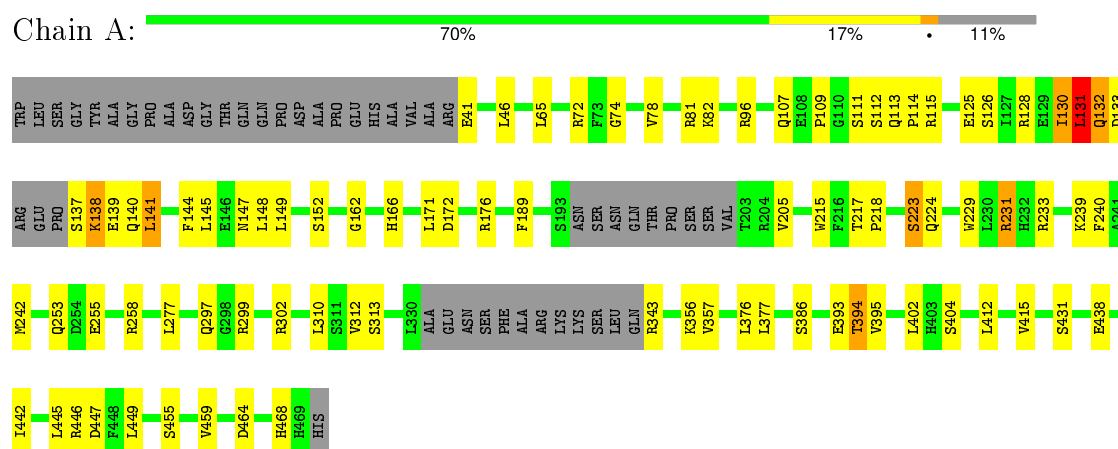
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	219	Total	O	0	0
			219	219		
4	B	245	Total	O	0	0
			245	245		
4	C	212	Total	O	0	0
			212	212		
4	D	206	Total	O	0	0
			206	206		

3 Residue-property plots

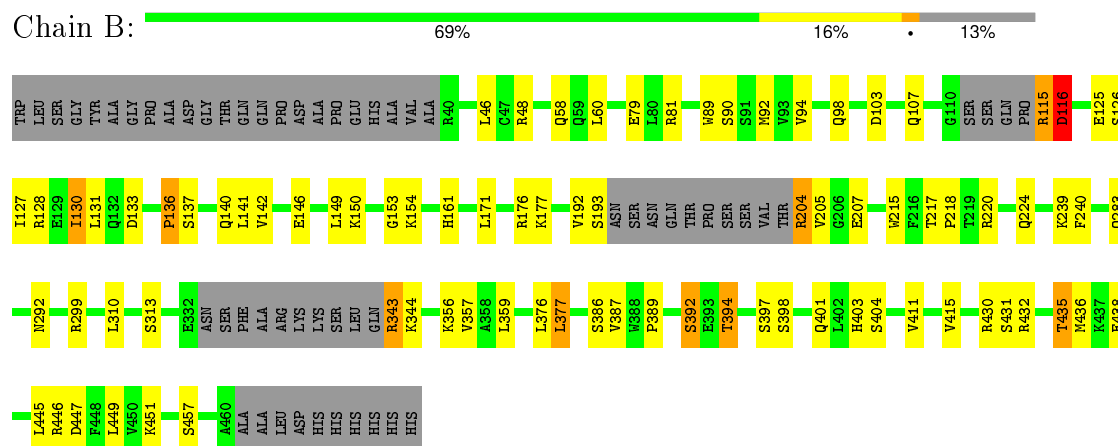
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

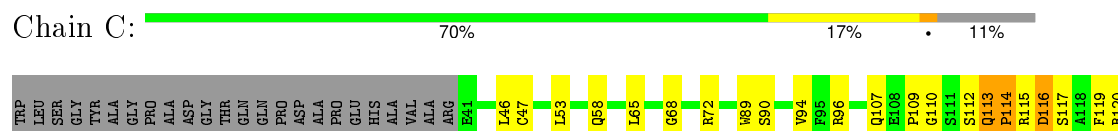
• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

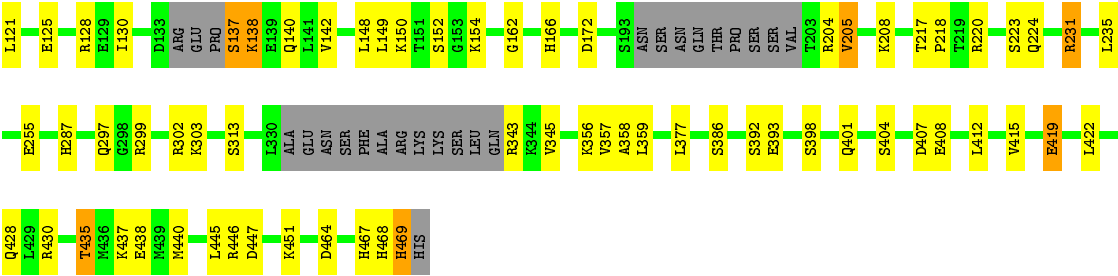


• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT

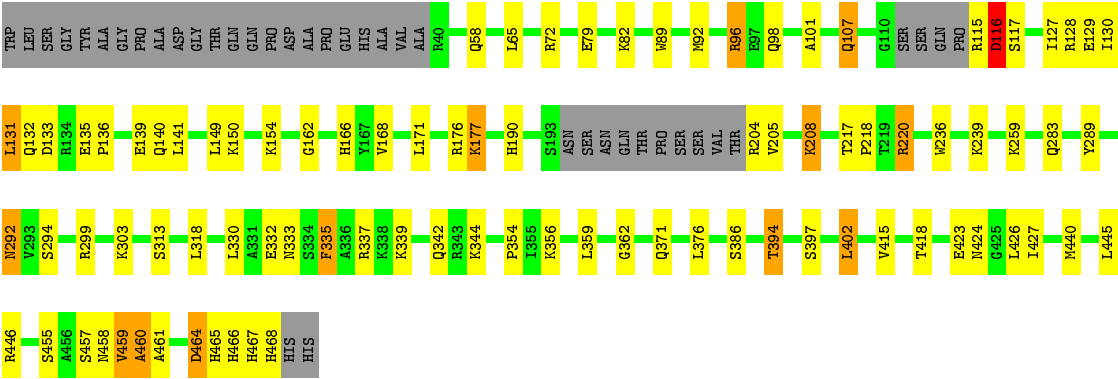


• Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT





● Molecule 1: MITOCHONDRIAL DNA POLYMERASE ACCESSORY SUBUNIT



4 Data and refinement statistics

Xtriage (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, α , β , γ	96.74Å 134.01Å 135.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (20.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13774	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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	0.34	0/3291	0.57	0/4461
1	B	0.34	0/3219	0.57	0/4362
1	C	0.32	0/3283	0.56	0/4450
1	D	0.33	0/3378	0.58	0/4576
All	All	0.34	0/13171	0.57	0/17849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3216	0	3206	62	0
1	B	3149	0	3154	60	0
1	C	3209	0	3194	66	0
1	D	3302	0	3300	69	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	0	0
4	A	219	0	0	5	0
4	B	245	0	0	13	0
4	C	212	0	0	8	0
4	D	206	0	0	6	0
All	All	13774	0	12870	226	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 9.

All (226) 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:A:109:PRO:HG3	1:D:58:GLN:HE21	1.20	1.03
1:D:466:HIS:HD2	1:D:468:HIS:H	1.25	0.82
1:A:138:LYS:HG3	1:B:136:PRO:HB2	1.62	0.80
1:A:231:ARG:HD2	1:A:468:HIS:HB3	1.64	0.80
1:A:128:ARG:HG3	1:B:149:LEU:HD21	1.63	0.79
1:C:430:ARG:NH2	1:C:435:THR:HG23	1.98	0.78
1:C:430:ARG:HH21	1:C:435:THR:HG23	1.50	0.77
1:B:430:ARG:NH2	1:B:435:THR:HG23	2.00	0.77
1:D:466:HIS:CD2	1:D:468:HIS:H	2.03	0.76
1:A:107:GLN:HE22	1:B:205:VAL:HG22	1.51	0.74
1:C:89:TRP:CD1	1:D:82:LYS:HE2	2.23	0.73
1:A:112:SER:HB2	1:A:149:LEU:O	1.88	0.73
1:B:58:GLN:HE21	1:C:109:PRO:HG3	1.54	0.72
1:B:58:GLN:HE22	1:D:204:ARG:NH2	1.86	0.72
1:C:113:GLN:HB3	1:C:114:PRO:HD3	1.71	0.71
1:D:204:ARG:HD2	4:D:971:HOH:O	1.92	0.69
1:C:58:GLN:HG3	4:C:1030:HOH:O	1.94	0.68
1:D:415:VAL:HG21	1:D:445:LEU:HD21	1.75	0.68
1:C:112:SER:OG	1:C:150:LYS:HG2	1.94	0.67
1:D:332:GLU:HG2	1:D:342:GLN:HG3	1.76	0.67
1:B:115:ARG:HG3	1:B:116:ASP:H	1.60	0.67
1:D:330:LEU:HD12	1:D:344:LYS:HG2	1.77	0.67
1:B:115:ARG:HA	1:B:154:LYS:HD2	1.77	0.67
1:D:458:ASN:O	1:D:459:VAL:C	2.34	0.66
1:D:135:GLU:N	1:D:136:PRO:HD3	2.11	0.65
1:A:109:PRO:HG3	1:D:58:GLN:NE2	2.03	0.64
1:B:81:ARG:HD2	4:B:919:HOH:O	1.99	0.63
1:B:299:ARG:HG2	4:B:1127:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLN:HB2	4:B:1094:HOH:O	2.00	0.62
1:B:343:ARG:HD3	4:B:995:HOH:O	2.00	0.62
1:D:376:LEU:HD21	1:D:445:LEU:HD23	1.80	0.62
1:A:224:GLN:HG3	4:A:954:HOH:O	1.99	0.62
1:C:162:GLY:O	1:C:166:HIS:HD2	1.83	0.61
1:C:467:HIS:CG	1:C:468:HIS:H	2.19	0.61
1:B:204:ARG:HA	4:B:1024:HOH:O	2.01	0.60
1:A:126:SER:O	1:A:130:ILE:HG23	2.01	0.60
1:A:82:LYS:HE2	1:B:89:TRP:NE1	2.16	0.60
1:C:142:VAL:HG23	1:D:141:LEU:HD11	1.84	0.59
1:B:283:GLN:HB2	4:B:997:HOH:O	2.01	0.59
1:B:153:GLY:HA3	4:B:1147:HOH:O	2.02	0.59
1:D:190:HIS:HB3	4:D:1028:HOH:O	2.01	0.59
1:C:65:LEU:O	1:C:72:ARG:HD3	2.03	0.59
1:D:236:TRP:O	1:D:239:LYS:HG2	2.03	0.58
1:C:107:GLN:HE22	1:D:205:VAL:HG22	1.67	0.58
1:B:136:PRO:O	1:B:137:SER:HB3	2.04	0.58
1:D:459:VAL:HG12	1:D:459:VAL:O	2.04	0.57
1:A:46:LEU:C	1:A:46:LEU:HD23	2.24	0.57
1:A:144:PHE:HA	1:A:147:ASN:HD22	1.69	0.57
1:D:459:VAL:HG11	1:D:466:HIS:CE1	2.39	0.57
1:D:424:ASN:OD1	1:D:426:LEU:HG	2.05	0.57
1:D:292:ASN:HD21	1:D:294:SER:CB	2.17	0.57
1:A:231:ARG:HD2	1:A:468:HIS:CB	2.35	0.56
1:C:447:ASP:HB3	1:C:451:LYS:NZ	2.20	0.56
1:C:113:GLN:CB	1:C:114:PRO:HD3	2.34	0.56
1:B:415:VAL:HG21	1:B:445:LEU:HD21	1.87	0.56
1:A:113:GLN:HB2	1:A:114:PRO:HD3	1.88	0.55
1:A:162:GLY:O	1:A:166:HIS:HD2	1.89	0.55
1:C:231:ARG:HG2	1:C:469:HIS:HB3	1.89	0.55
1:A:217:THR:OG1	1:A:218:PRO:HD2	2.07	0.55
1:C:148:LEU:O	1:C:152:SER:HB2	2.07	0.55
1:C:356:LYS:O	1:C:412:LEU:HB2	2.07	0.54
1:C:138:LYS:HE2	1:D:136:PRO:O	2.06	0.54
1:B:115:ARG:N	1:B:154:LYS:HZ3	2.05	0.54
1:C:467:HIS:CG	1:C:468:HIS:N	2.75	0.54
1:B:430:ARG:HH21	1:B:435:THR:HG23	1.68	0.54
1:D:171:LEU:CD1	1:D:176:ARG:HA	2.37	0.54
1:C:440:MET:HE1	1:C:445:LEU:HA	1.90	0.54
1:A:376:LEU:HD22	1:A:442:ILE:HD11	1.90	0.54
1:A:231:ARG:HD2	1:A:468:HIS:CG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG21	1:A:445:LEU:HD21	1.90	0.53
1:A:231:ARG:CD	1:A:468:HIS:ND1	2.72	0.53
1:D:330:LEU:HD21	1:D:342:GLN:HG2	1.90	0.53
1:A:82:LYS:HE2	1:B:89:TRP:CD1	2.43	0.53
1:C:356:LYS:HG2	1:C:386:SER:OG	2.08	0.53
1:D:362:GLY:HA3	1:D:418:THR:HG22	1.91	0.53
1:A:130:ILE:HG13	1:A:131:LEU:N	2.24	0.53
1:A:138:LYS:CG	1:B:136:PRO:HB2	2.36	0.53
1:D:458:ASN:O	1:D:460:ALA:N	2.42	0.53
1:C:107:GLN:NE2	1:D:205:VAL:HG22	2.24	0.53
1:A:223:SER:HB2	4:A:990:HOH:O	2.09	0.53
1:C:112:SER:HB3	1:C:149:LEU:O	2.09	0.52
1:A:395:VAL:O	1:A:395:VAL:HG23	2.10	0.52
1:B:127:ILE:O	1:B:130:ILE:HG22	2.09	0.52
1:D:283:GLN:HB2	4:D:949:HOH:O	2.08	0.52
1:C:217:THR:OG1	1:C:218:PRO:HD2	2.09	0.52
1:C:231:ARG:CD	1:C:469:HIS:HB3	2.39	0.52
1:C:116:ASP:OD2	1:C:154:LYS:HE2	2.10	0.51
1:D:356:LYS:HG2	1:D:386:SER:OG	2.09	0.51
1:C:235:LEU:HG	4:C:992:HOH:O	2.09	0.51
1:C:231:ARG:CG	1:C:469:HIS:HB3	2.40	0.51
1:C:47:CYS:HB3	1:C:53:LEU:HG	1.93	0.51
1:C:46:LEU:C	1:C:46:LEU:HD23	2.31	0.51
1:C:90:SER:HA	1:C:94:VAL:HB	1.92	0.51
1:B:359:LEU:HD23	1:B:415:VAL:HB	1.93	0.51
1:A:107:GLN:HG2	1:B:207:GLU:OE2	2.11	0.50
1:B:215:TRP:HB3	1:B:310:LEU:HB2	1.93	0.50
1:C:137:SER:HB2	1:C:140:GLN:HG3	1.94	0.50
1:B:171:LEU:CD1	1:B:176:ARG:HA	2.42	0.50
1:C:287:HIS:HB2	4:C:1105:HOH:O	2.12	0.50
1:A:145:LEU:HD13	1:B:130:ILE:HG21	1.93	0.50
1:C:231:ARG:HG2	1:C:469:HIS:C	2.31	0.50
1:C:128:ARG:HH11	1:C:128:ARG:HG2	1.76	0.50
1:A:356:LYS:HG2	1:A:386:SER:OG	2.11	0.50
1:D:460:ALA:O	1:D:464:ASP:N	2.45	0.50
1:B:115:ARG:CG	1:B:116:ASP:H	2.24	0.50
1:C:430:ARG:HH21	1:C:435:THR:CG2	2.20	0.49
1:D:333:ASN:OD1	1:D:335:PHE:HB3	2.12	0.49
1:B:403:HIS:CE1	1:B:430:ARG:HD2	2.47	0.49
1:D:461:ALA:O	1:D:464:ASP:HB2	2.13	0.49
1:A:393:GLU:HG3	1:A:394:THR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:NZ	1:B:136:PRO:HG3	2.27	0.48
1:B:447:ASP:HB3	1:B:451:LYS:NZ	2.27	0.48
1:A:231:ARG:HD3	1:A:468:HIS:ND1	2.28	0.48
1:D:440:MET:HE1	1:D:445:LEU:HA	1.95	0.48
1:C:359:LEU:HD23	1:C:415:VAL:HB	1.95	0.48
1:C:393:GLU:OE2	1:D:177:LYS:HE2	2.14	0.48
1:C:205:VAL:CG1	1:D:107:GLN:HE22	2.27	0.48
1:B:411:VAL:O	1:B:432:ARG:HB2	2.14	0.48
1:D:459:VAL:HG11	1:D:466:HIS:HE1	1.77	0.48
1:C:113:GLN:HB3	1:C:114:PRO:CD	2.42	0.48
1:C:116:ASP:O	1:C:117:SER:CB	2.62	0.48
1:A:357:VAL:HG11	1:A:449:LEU:CD1	2.44	0.48
1:A:171:LEU:HD12	1:A:176:ARG:HA	1.96	0.47
1:B:356:LYS:HG2	1:B:386:SER:OG	2.14	0.47
1:B:357:VAL:HG21	1:B:449:LEU:HD13	1.95	0.47
1:B:239:LYS:HE3	1:B:240:PHE:CZ	2.49	0.47
1:A:112:SER:OG	1:A:149:LEU:HG	2.14	0.47
1:C:116:ASP:O	1:C:117:SER:HB3	2.15	0.47
1:D:115:ARG:N	1:D:154:LYS:HZ2	2.12	0.47
1:C:357:VAL:HG12	1:C:358:ALA:N	2.29	0.47
1:C:404:SER:O	1:C:408:GLU:HG3	2.15	0.47
1:C:419:GLU:O	1:C:422:LEU:HB2	2.15	0.47
1:C:107:GLN:HG2	1:C:121:LEU:CD1	2.45	0.47
1:D:466:HIS:HD2	1:D:468:HIS:N	2.03	0.46
1:A:138:LYS:HG2	1:A:138:LYS:O	2.15	0.46
1:A:231:ARG:HD2	1:A:468:HIS:ND1	2.29	0.46
1:B:377:LEU:HD12	1:B:387:VAL:CG1	2.45	0.46
1:A:239:LYS:HE3	1:A:240:PHE:CZ	2.51	0.46
1:A:394:THR:O	1:A:395:VAL:HG22	2.15	0.46
1:A:172:ASP:HB2	4:C:1003:HOH:O	2.14	0.46
1:D:359:LEU:HD23	1:D:415:VAL:HB	1.98	0.46
1:C:130:ILE:HG12	1:C:130:ILE:O	2.15	0.46
1:A:447:ASP:HB3	4:A:1091:HOH:O	2.15	0.46
1:B:398:SER:OG	1:B:401:GLN:HG3	2.15	0.46
1:B:46:LEU:HD23	1:B:46:LEU:C	2.36	0.46
1:B:137:SER:HB3	1:B:140:GLN:OE1	2.17	0.45
1:A:299:ARG:HH22	1:B:394:THR:HB	1.80	0.45
1:B:217:THR:OG1	1:B:218:PRO:HD2	2.16	0.45
1:A:148:LEU:O	1:A:152:SER:HB2	2.16	0.45
1:C:345:VAL:HG23	1:C:407:ASP:HB3	1.99	0.45
1:D:217:THR:OG1	1:D:218:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD12	1:B:141:LEU:HB2	1.98	0.45
1:C:224:GLN:HG3	4:C:941:HOH:O	2.16	0.45
1:D:98:GLN:HB2	4:D:1067:HOH:O	2.17	0.45
1:B:58:GLN:HE22	1:D:204:ARG:HH22	1.58	0.45
1:C:137:SER:OG	1:C:140:GLN:NE2	2.50	0.45
1:A:141:LEU:HD12	1:B:141:LEU:CB	2.47	0.45
1:D:318:LEU:HA	1:D:318:LEU:HD12	1.75	0.45
1:D:79:GLU:HB3	1:D:354:PRO:HB3	1.99	0.45
1:A:189:PHE:N	1:A:189:PHE:CD1	2.85	0.45
1:A:115:ARG:HD2	4:B:1143:HOH:O	2.16	0.45
1:D:467:HIS:O	1:D:468:HIS:HB2	2.17	0.44
1:B:292:ASN:HA	4:B:1142:HOH:O	2.18	0.44
1:D:402:LEU:HD12	1:D:402:LEU:HA	1.86	0.44
1:A:74:GLY:O	1:A:78:VAL:HG23	2.17	0.44
1:D:464:ASP:HB3	1:D:465:HIS:CD2	2.53	0.44
1:C:428:GLN:NE2	1:C:437:LYS:HD3	2.32	0.44
1:C:68:GLY:HA2	4:C:974:HOH:O	2.17	0.44
1:D:89:TRP:HZ2	1:D:101:ALA:HB2	1.83	0.44
1:B:79:GLU:HG3	4:B:1082:HOH:O	2.18	0.44
1:B:224:GLN:HG3	4:B:927:HOH:O	2.17	0.44
1:A:131:LEU:O	1:A:133:ASP:N	2.51	0.44
1:C:149:LEU:HD21	1:D:128:ARG:HG3	2.00	0.44
1:D:427:ILE:HD12	1:D:427:ILE:O	2.17	0.44
1:D:132:GLN:HG3	4:D:1042:HOH:O	2.17	0.44
1:B:376:LEU:HD21	1:B:445:LEU:HD23	2.00	0.44
1:A:242:MET:HB3	1:A:242:MET:HE2	1.84	0.44
1:A:149:LEU:HD21	1:B:128:ARG:HG3	1.98	0.44
1:D:107:GLN:HG2	1:D:107:GLN:O	2.18	0.44
1:D:190:HIS:O	1:D:190:HIS:CD2	2.71	0.43
1:A:297:GLN:HB2	4:A:938:HOH:O	2.18	0.43
1:D:162:GLY:O	1:D:166:HIS:HD2	2.02	0.43
1:D:168:VAL:HG23	1:D:289:TYR:CZ	2.53	0.43
1:A:65:LEU:O	1:A:72:ARG:HD3	2.19	0.43
1:B:377:LEU:HD12	1:B:387:VAL:HG11	2.01	0.43
1:D:208:LYS:O	1:D:208:LYS:HG3	2.18	0.43
1:C:299:ARG:NH2	1:D:394:THR:OG1	2.52	0.43
1:C:119:PHE:HD1	4:C:1012:HOH:O	2.02	0.43
1:D:65:LEU:O	1:D:72:ARG:HD3	2.19	0.42
1:B:115:ARG:HB3	1:B:154:LYS:HE2	2.01	0.42
1:D:135:GLU:N	1:D:136:PRO:CD	2.81	0.42
1:D:116:ASP:HB3	1:D:117:SER:H	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASP:HB3	1:C:120:ARG:HH12	1.84	0.42
1:C:114:PRO:HB2	1:C:115:ARG:H	1.68	0.42
1:C:107:GLN:HG2	1:C:121:LEU:HD11	2.01	0.42
1:C:297:GLN:HB2	4:C:946:HOH:O	2.19	0.42
1:C:398:SER:OG	1:C:401:GLN:HG3	2.19	0.42
4:A:966:HOH:O	1:C:172:ASP:HB2	2.18	0.42
1:A:253:GLN:HA	1:A:258:ARG:O	2.19	0.42
1:D:96:ARG:HE	1:D:96:ARG:HB3	1.79	0.42
1:B:161:HIS:HD2	4:B:1069:HOH:O	2.02	0.42
1:C:149:LEU:HD13	1:D:127:ILE:HG21	2.01	0.42
1:C:205:VAL:HG12	1:D:107:GLN:OE1	2.19	0.41
1:A:402:LEU:HA	1:A:402:LEU:HD12	1.92	0.41
1:D:131:LEU:HA	1:D:131:LEU:HD12	1.89	0.41
1:B:447:ASP:HB3	1:B:451:LYS:HZ3	1.85	0.41
1:A:81:ARG:HH22	1:B:103:ASP:CG	2.23	0.41
1:A:356:LYS:O	1:A:412:LEU:HB2	2.21	0.41
1:D:427:ILE:C	1:D:427:ILE:HD12	2.40	0.41
1:D:176:ARG:HB2	1:D:299:ARG:HD3	2.01	0.41
1:A:229:TRP:O	1:A:233:ARG:HG2	2.20	0.41
1:C:89:TRP:NE1	1:D:82:LYS:HE2	2.34	0.41
1:B:58:GLN:HG3	4:B:1070:HOH:O	2.21	0.41
1:C:110:GLY:HA3	1:C:152:SER:O	2.21	0.41
1:B:142:VAL:O	1:B:146:GLU:HB2	2.21	0.41
1:D:459:VAL:CG1	1:D:466:HIS:CE1	3.03	0.41
1:A:455:SER:O	1:A:459:VAL:HG23	2.21	0.41
1:A:215:TRP:HB3	1:A:310:LEU:HB2	2.02	0.40
1:A:111:SER:C	1:A:113:GLN:H	2.24	0.40
1:A:41:GLU:HG3	1:A:41:GLU:O	2.20	0.40
1:B:389:PRO:O	1:B:392:SER:HB2	2.21	0.40
1:C:438:GLU:HG3	1:C:438:GLU:O	2.20	0.40
1:A:277:LEU:HG	1:A:312:VAL:HG13	2.02	0.40
1:B:90:SER:HA	1:B:94:VAL:HB	2.03	0.40
1:B:48:ARG:HG2	1:B:60:LEU:HD11	2.04	0.40
1:D:220:ARG:HB3	4:D:980:HOH:O	2.22	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%)	381 (96%)	14 (4%)	2 (0%)	34	41
1	B	389/454 (86%)	377 (97%)	10 (3%)	2 (0%)	34	41
1	C	397/454 (87%)	385 (97%)	10 (2%)	2 (0%)	34	41
1	D	409/454 (90%)	392 (96%)	14 (3%)	3 (1%)	26	31
All	All	1592/1816 (88%)	1535 (96%)	48 (3%)	9 (1%)	30	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	PRO
1	D	116	ASP
1	D	459	VAL
1	D	460	ALA
1	C	114	PRO
1	B	116	ASP
1	A	131	LEU
1	A	132	GLN
1	C	116	ASP

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	357/397 (90%)	333 (93%)	24 (7%)	20	26
1	B	349/397 (88%)	320 (92%)	29 (8%)	14	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	355/397 (89%)	332 (94%)	23 (6%)	21	27
1	D	365/397 (92%)	334 (92%)	31 (8%)	13	16
All	All	1426/1588 (90%)	1319 (92%)	107 (8%)	17	21

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	125	GLU
1	A	130	ILE
1	A	131	LEU
1	A	132	GLN
1	A	137	SER
1	A	138	LYS
1	A	139	GLU
1	A	140	GLN
1	A	141	LEU
1	A	205	VAL
1	A	223	SER
1	A	231	ARG
1	A	255	GLU
1	A	302	ARG
1	A	313	SER
1	A	343	ARG
1	A	377	LEU
1	A	394	THR
1	A	404	SER
1	A	431	SER
1	A	438	GLU
1	A	446	ARG
1	A	464	ASP
1	B	92	MET
1	B	107	GLN
1	B	115	ARG
1	B	116	ASP
1	B	125	GLU
1	B	126	SER
1	B	130	ILE
1	B	131	LEU
1	B	133	ASP
1	B	150	LYS

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Mol	Chain	Res	Type
1	B	177	LYS
1	B	192	VAL
1	B	193	SER
1	B	204	ARG
1	B	220	ARG
1	B	313	SER
1	B	343	ARG
1	B	344	LYS
1	B	377	LEU
1	B	392	SER
1	B	394	THR
1	B	397	SER
1	B	404	SER
1	B	431	SER
1	B	435	THR
1	B	436	MET
1	B	438	GLU
1	B	446	ARG
1	B	457	SER
1	C	96	ARG
1	C	113	GLN
1	C	125	GLU
1	C	137	SER
1	C	138	LYS
1	C	204	ARG
1	C	205	VAL
1	C	208	LYS
1	C	220	ARG
1	C	223	SER
1	C	231	ARG
1	C	255	GLU
1	C	302	ARG
1	C	303	LYS
1	C	313	SER
1	C	343	ARG
1	C	377	LEU
1	C	392	SER
1	C	419	GLU
1	C	435	THR
1	C	446	ARG
1	C	464	ASP
1	C	469	HIS

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Mol	Chain	Res	Type
1	D	92	MET
1	D	96	ARG
1	D	107	GLN
1	D	116	ASP
1	D	129	GLU
1	D	130	ILE
1	D	131	LEU
1	D	133	ASP
1	D	139	GLU
1	D	140	GLN
1	D	149	LEU
1	D	150	LYS
1	D	177	LYS
1	D	208	LYS
1	D	220	ARG
1	D	259	LYS
1	D	292	ASN
1	D	303	LYS
1	D	313	SER
1	D	335	PHE
1	D	337	ARG
1	D	339	LYS
1	D	371	GLN
1	D	394	THR
1	D	397	SER
1	D	402	LEU
1	D	423	GLU
1	D	446	ARG
1	D	455	SER
1	D	457	SER
1	D	464	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	113	GLN
1	A	147	ASN
1	A	166	HIS
1	A	292	ASN
1	A	329	GLN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	190	HIS
1	B	371	GLN
1	B	374	GLN
1	C	140	GLN
1	C	166	HIS
1	C	374	GLN
1	C	383	ASN
1	C	465	HIS
1	C	467	HIS
1	D	58	GLN
1	D	166	HIS
1	D	292	ASN
1	D	374	GLN
1	D	466	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 carbohydrates 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	B	6	-	5,5,5	0.31	0	5,5,5	0.37	0
3	GOL	D	5	-	5,5,5	0.31	0	5,5,5	0.40	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.

No monomer is involved in short contacts.

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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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