Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:40 PM EST

PDB ID	:	1M0T
Title	:	Yeast Glutathione Synthase
Authors	:	Gogos, A.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2002-06-14
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
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:

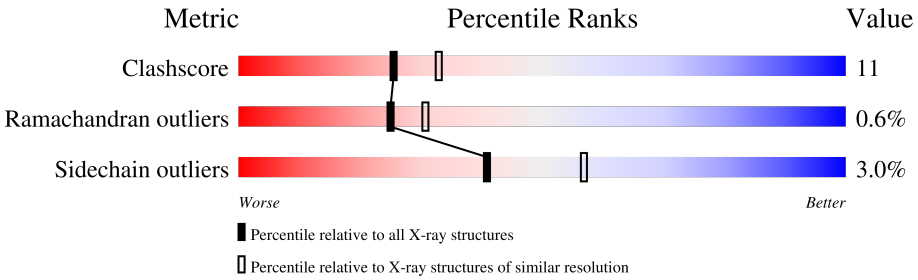
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	72% 19% • 8%
1	B	491	74% 16% • 7%

2 Entry composition

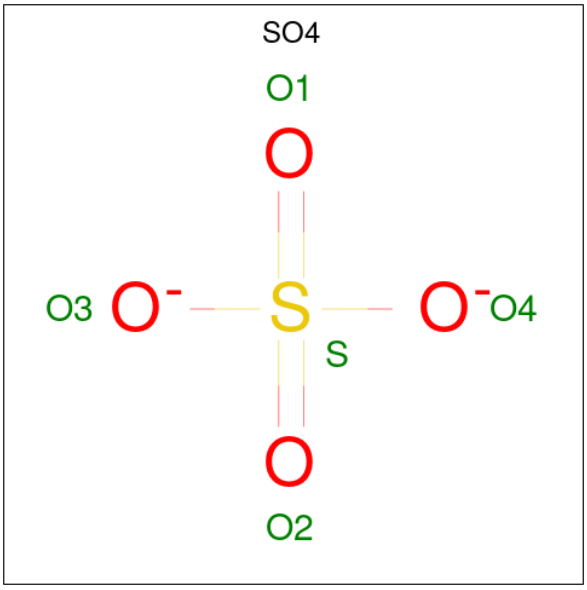
There are 3 unique types of molecules in this entry. The entry contains 7979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glutathione synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	21	0
			3761	2406	614	733	8			
1	B	455	Total	C	N	O	S	0	15	0
			3690	2375	603	703	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	265	Total O 265 265	0	0
3	B	233	Total O 233 233	0	0

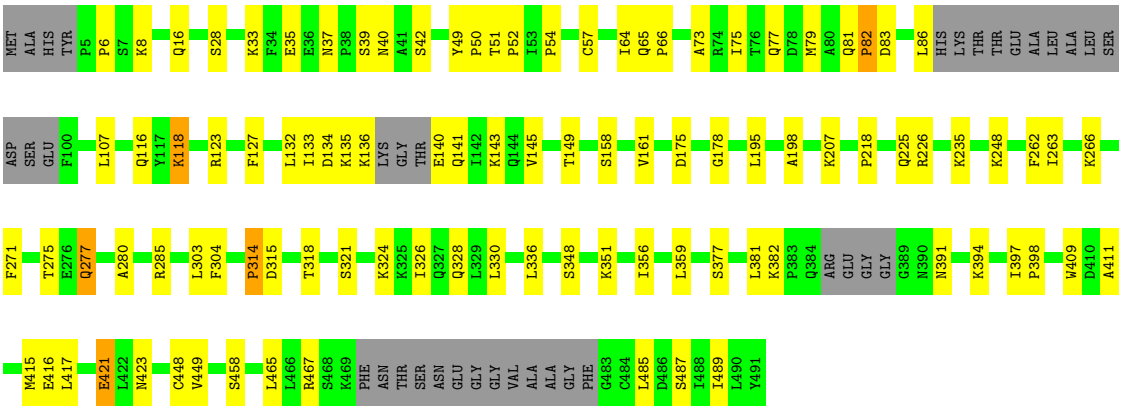
3 Residue-property plots (i)

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.

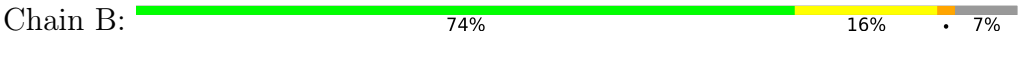
• Molecule 1: glutathione synthetase

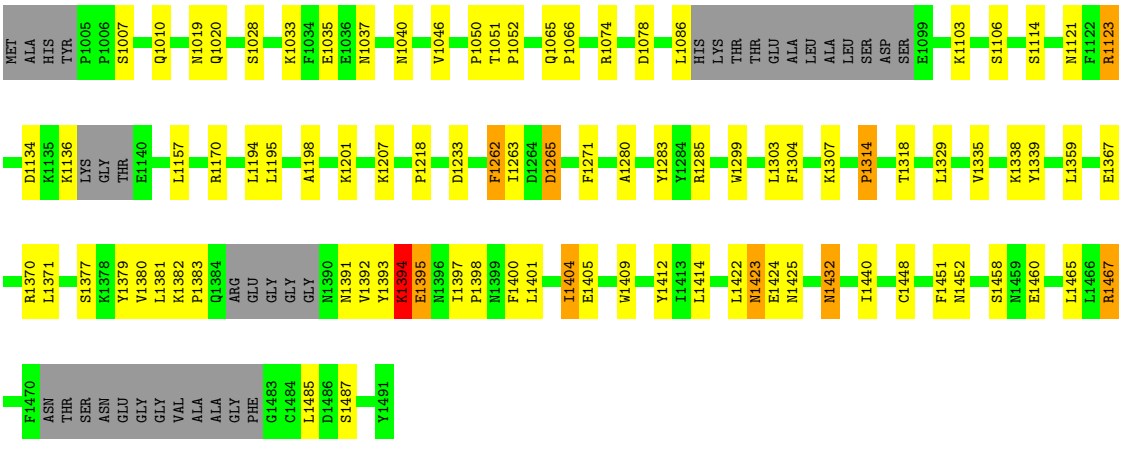
Chain A:



• Molecule 1: glutathione synthetase

Chain B:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.87Å 155.07Å 190.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.2 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.216 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7979	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.53	0/3831	0.65	0/5188
1	B	0.49	0/3760	0.63	0/5091
All	All	0.51	0/7591	0.64	0/10279

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

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	3761	0	3655	82	0
1	B	3690	0	3582	82	0
2	A	10	0	0	1	0
2	B	20	0	0	0	0
3	A	265	0	0	2	0
3	B	233	0	0	3	0
All	All	7979	0	7237	157	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 (157) 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:135:LYS:HE2	1:A:140:GLU:HG2	1.42	0.99
1:B:1422:LEU:HD13	1:B:1440[A]:ILE:HD11	1.44	0.96
1:B:1422:LEU:CD1	1:B:1440[A]:ILE:CD1	2.45	0.94
1:B:1404:ILE:HG22	1:B:1405:GLU:H	1.31	0.93
1:B:1422:LEU:CD1	1:B:1440[A]:ILE:HD11	2.00	0.90
1:B:1019:ASN:HD21	1:B:1432:ASN:HD21	1.19	0.90
1:B:1422:LEU:HD12	1:B:1440[A]:ILE:HD13	1.56	0.87
1:A:40[A]:ASN:HD21	1:B:1040[A]:ASN:HD22	1.20	0.86
1:B:1422:LEU:HD12	1:B:1440[A]:ILE:CD1	2.05	0.86
1:B:1465:LEU:HD21	1:B:1467:ARG:HD3	1.57	0.86
1:A:123:ARG:HD3	1:A:315:ASP:OD1	1.79	0.82
1:A:79:MET:HE1	1:A:321:SER:HA	1.61	0.82
1:B:1359:LEU:HD11	1:B:1381:LEU:HD11	1.64	0.80
1:A:277[A]:GLN:HE21	1:A:277[A]:GLN:HA	1.49	0.78
1:A:467:ARG:NH1	2:A:504:SO4:O3	2.21	0.74
1:B:1467:ARG:HG3	1:B:1467:ARG:HH11	1.52	0.74
1:B:1198:ALA:HB1	1:B:1448[B]:CYS:SG	2.29	0.72
1:B:1198:ALA:O	1:B:1201[A]:LYS:HG2	1.90	0.72
1:A:356:ILE:HG12	1:A:415:MET:HG3	1.72	0.71
1:B:1033:LYS:HA	1:B:1035:GLU:OE1	1.90	0.71
1:A:141:GLN:OE1	1:A:351[A]:LYS:HE3	1.92	0.70
1:A:382:LYS:HD2	1:A:415:MET:HE3	1.73	0.70
1:A:82:PRO:HD3	3:A:2437:HOH:O	1.92	0.69
1:A:40[A]:ASN:HD21	1:B:1040[A]:ASN:ND2	1.91	0.69
1:B:1019:ASN:ND2	1:B:1432:ASN:HD21	1.92	0.67
1:B:1218:PRO:HB2	1:B:1280:ALA:HB2	1.78	0.66
1:A:377:SER:HA	1:A:394:LYS:HB3	1.79	0.65
1:A:116:GLN:HE21	1:A:266:LYS:HA	1.61	0.64
1:A:465:LEU:HD21	1:A:467:ARG:HD3	1.80	0.64
1:A:132:LEU:HD12	1:A:145[B]:VAL:HG11	1.80	0.63
1:A:143:LYS:HE3	1:A:416[A]:GLU:OE2	2.00	0.62
1:A:218:PRO:HB2	1:A:280:ALA:HB2	1.83	0.60
1:B:1086:LEU:HD22	1:B:1339:TYR:OH	2.01	0.60
1:B:1404:ILE:HG22	1:B:1405:GLU:N	2.10	0.60
1:B:1401:LEU:HB3	1:B:1409:TRP:CZ2	2.36	0.59
1:B:1019:ASN:HD21	1:B:1432:ASN:ND2	1.95	0.59
1:A:33:LYS:HA	1:A:35:GLU:OE1	2.01	0.59
1:A:123:ARG:HG3	1:A:123:ARG:NH1	2.17	0.59
1:A:314:PRO:HB2	1:A:318:THR:HB	1.85	0.59
1:B:1382:LYS:HG2	1:B:1391:ASN:OD1	2.03	0.58
1:A:277[A]:GLN:NE2	1:A:277[A]:GLN:HA	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:GLN:HB3	1:B:1066:PRO:HD3	1.87	0.57
1:B:1359:LEU:CD1	1:B:1381:LEU:HD11	2.34	0.57
1:A:277[A]:GLN:CA	1:A:277[A]:GLN:HE21	2.11	0.57
1:A:198:ALA:HB1	1:A:448[B]:CYS:SG	2.45	0.56
1:B:1123:ARG:HD3	1:B:1451:PHE:CE1	2.40	0.56
1:A:86:LEU:HD11	1:A:326:ILE:HG23	1.88	0.56
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.70	0.54
1:B:1382:LYS:HG2	1:B:1391:ASN:CG	2.26	0.54
1:B:1423:ASN:ND2	1:B:1425:ASN:H	2.05	0.54
1:B:1157:LEU:HG	1:B:1233:ASP:HB2	1.88	0.54
1:A:382:LYS:HD2	1:A:415:MET:CE	2.37	0.54
1:A:118:LYS:HD2	1:A:118:LYS:H	1.73	0.53
1:A:65:GLN:HB3	1:A:66:PRO:HD3	1.89	0.53
1:B:1381:LEU:HD21	1:B:1401:LEU:HD21	1.92	0.52
1:A:40[A]:ASN:ND2	1:B:1040[A]:ASN:HD22	1.99	0.52
1:B:1035:GLU:H	1:B:1035:GLU:CD	2.13	0.52
1:B:1467:ARG:HG3	1:B:1467:ARG:NH1	2.23	0.52
1:B:1314:PRO:HB2	1:B:1318:THR:HB	1.91	0.51
1:A:54:PRO:HG2	1:A:57:CYS:HB2	1.92	0.51
1:B:1265:ASP:N	1:B:1265:ASP:OD1	2.43	0.51
1:B:1207:LYS:HD2	1:B:1218:PRO:HD2	1.91	0.51
1:B:1123:ARG:HB2	3:B:2092:HOH:O	2.10	0.50
1:A:132:LEU:CD1	1:A:145[B]:VAL:HG11	2.42	0.50
1:A:275:THR:OG1	1:A:277[B]:GLN:HG3	2.11	0.50
1:A:135:LYS:CE	1:A:140:GLU:HG2	2.28	0.50
1:A:123:ARG:HD3	1:A:315:ASP:CG	2.32	0.49
1:A:263:ILE:HG13	1:A:304:PHE:CZ	2.47	0.49
1:B:1367:GLU:O	1:B:1371:LEU:HG	2.14	0.48
1:A:324:LYS:O	1:A:328:GLN:HG3	2.14	0.48
1:A:262:PHE:CE2	1:A:271:PHE:HB2	2.49	0.48
1:A:42:SER:OG	1:B:1040[A]:ASN:ND2	2.47	0.48
1:B:1263:ILE:HG13	1:B:1304:PHE:CZ	2.49	0.48
1:A:52:PRO:HA	1:A:489:ILE:HG23	1.95	0.48
1:A:207:LYS:HG2	1:A:218:PRO:HG3	1.96	0.47
1:B:1201[B]:LYS:HE3	1:B:1458:SER:HB2	1.96	0.47
1:A:421[A]:GLU:HG3	1:A:421[A]:GLU:H	1.39	0.47
1:A:75:ILE:HG22	1:A:79:MET:HE2	1.95	0.47
1:A:134:ASP:OD1	1:A:136:LYS:HG3	2.14	0.47
1:B:1465:LEU:HD21	1:B:1467:ARG:CD	2.39	0.47
1:A:75:ILE:HG22	1:A:79:MET:CE	2.44	0.47
1:B:1194:LEU:HD22	3:B:2496:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1134:ASP:OD2	1:B:1136:LYS:HE2	2.15	0.47
1:B:1198:ALA:HA	1:B:1201[A]:LYS:HE2	1.97	0.46
1:B:1303:LEU:HD11	1:B:1307:LYS:HE3	1.98	0.46
1:B:1262:PHE:CE2	1:B:1271:PHE:HB2	2.50	0.46
1:A:127:PHE:CD2	1:A:149:THR:HA	2.51	0.46
1:B:1397:ILE:HB	1:B:1398:PRO:HD3	1.97	0.46
1:A:123:ARG:CG	1:A:123:ARG:HH11	2.29	0.46
1:B:1103:LYS:O	1:B:1106:SER:HB3	2.15	0.46
1:B:1422:LEU:HD11	1:B:1440[A]:ILE:HG12	1.96	0.46
1:B:1198:ALA:CB	1:B:1448[B]:CYS:SG	3.02	0.46
1:B:1285:ARG:HA	1:B:1285:ARG:HD2	1.81	0.46
1:B:1422:LEU:CD1	1:B:1440[A]:ILE:CG1	2.93	0.46
1:A:35:GLU:H	1:A:35:GLU:CD	2.19	0.45
1:B:1074:ARG:NH1	1:B:1339:TYR:O	2.42	0.45
1:B:1377:SER:OG	1:B:1395:GLU:HG3	2.16	0.45
1:A:107:LEU:HD22	1:A:303:LEU:HB2	1.98	0.45
1:B:1392:VAL:HG21	1:B:1400:PHE:CG	2.51	0.45
1:A:81:GLN:C	1:A:83:ASP:H	2.19	0.45
1:B:1400:PHE:HZ	1:B:1412:TYR:HH	1.63	0.45
1:B:1367:GLU:HA	1:B:1370:ARG:HD2	1.99	0.45
1:A:54:PRO:HG2	1:A:57:CYS:SG	2.56	0.45
1:B:1401:LEU:HB3	1:B:1409:TRP:CE2	2.52	0.45
1:B:1123:ARG:HG3	1:B:1451:PHE:CZ	2.52	0.44
1:A:449:VAL:HA	1:A:458:SER:O	2.16	0.44
1:A:133:ILE:HB	1:A:421[A]:GLU:CG	2.48	0.44
1:A:359:LEU:HD11	1:A:381:LEU:HD11	1.99	0.44
1:B:1440[A]:ILE:HD13	1:B:1440[A]:ILE:HA	1.86	0.44
1:A:397:ILE:HB	1:A:398:PRO:HD3	1.98	0.44
1:B:1379:TYR:HB2	1:B:1414:LEU:HD11	1.99	0.44
1:B:1123:ARG:NH2	3:B:2151:HOH:O	2.50	0.44
1:A:225:GLN:HG2	1:A:226:ARG:O	2.18	0.43
1:B:1422:LEU:CD1	1:B:1440[A]:ILE:HG12	2.48	0.43
1:A:467:ARG:HB2	1:A:467:ARG:HE	1.61	0.43
1:B:1078:ASP:HB3	1:B:1086:LEU:HD23	1.99	0.43
1:A:248:LYS:HE3	1:B:1170:ARG:O	2.17	0.43
1:A:145[A]:VAL:O	1:A:145[A]:VAL:HG22	2.18	0.43
1:A:161[A]:VAL:HG21	1:A:485:LEU:HB3	2.01	0.43
1:A:64:ILE:HD13	1:A:348:SER:HB3	1.99	0.43
1:A:39[B]:SER:C	1:A:40[B]:ASN:HD22	2.22	0.43
1:A:161[A]:VAL:HG21	1:A:485:LEU:CB	2.49	0.43
1:B:1103:LYS:HG2	1:B:1299:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:SER:OG	1:B:1010[A]:GLN:HB2	2.19	0.42
1:A:235:LYS:NZ	1:B:1020:GLN:HE21	2.17	0.42
1:A:158:SER:O	1:A:161[B]:VAL:HG12	2.19	0.42
1:A:86:LEU:HD13	1:A:326:ILE:HG12	2.01	0.42
1:B:1394:LYS:HB3	1:B:1395:GLU:H	1.34	0.42
1:A:73:ALA:O	1:A:77:GLN:HG3	2.20	0.42
1:B:1381:LEU:HB3	1:B:1392:VAL:HB	2.02	0.42
1:A:75:ILE:CG2	1:A:79:MET:HE2	2.50	0.42
1:A:235:LYS:NZ	1:B:1020:GLN:NE2	2.68	0.42
1:B:1050:PRO:HB3	1:B:1487:SER:OG	2.20	0.42
1:B:1051:THR:HA	1:B:1052:PRO:HD3	1.88	0.41
1:B:1335:VAL:HA	1:B:1338:LYS:HD2	2.01	0.41
1:B:1359:LEU:HD11	1:B:1381:LEU:CD1	2.43	0.41
1:A:136:LYS:HD3	1:A:417:LEU:O	2.19	0.41
1:A:489:ILE:HG23	1:A:489:ILE:O	2.20	0.41
1:A:6:PRO:HG3	1:A:49:TYR:OH	2.20	0.41
1:A:75:ILE:HD11	1:A:330:LEU:HD21	2.03	0.41
1:A:81:GLN:O	1:A:83:ASP:N	2.53	0.41
1:B:1121:ASN:O	1:B:1452:ASN:HA	2.21	0.41
1:A:382:LYS:HG2	1:A:391:ASN:OD1	2.20	0.41
1:B:1134:ASP:OD1	1:B:1136:LYS:HG3	2.20	0.41
1:B:1382:LYS:HA	1:B:1383:PRO:HD3	1.87	0.41
1:A:16[B]:GLN:HG3	3:A:2057:HOH:O	2.20	0.41
1:A:409:TRP:C	1:A:411:ALA:H	2.25	0.41
1:B:1380:VAL:HG12	1:B:1393:TYR:CD2	2.56	0.41
1:B:1046:VAL:HG12	1:B:1485:LEU:HB2	2.02	0.40
1:A:285:ARG:HD2	1:A:285:ARG:HA	1.90	0.40
1:A:8:LYS:HD3	1:A:8:LYS:HA	1.88	0.40
1:A:40[B]:ASN:N	1:A:40[B]:ASN:HD22	2.19	0.40
1:A:50:PRO:HB3	1:A:487:SER:OG	2.21	0.40
1:A:51:THR:HA	1:A:52:PRO:HD3	1.90	0.40
1:A:175:ASP:HB3	1:A:178:GLY:O	2.22	0.40
1:B:1283:TYR:CZ	1:B:1285:ARG:HD3	2.57	0.40
1:B:1392:VAL:HG11	1:B:1400:PHE:CB	2.51	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	465/491 (95%)	450 (97%)	14 (3%)	1 (0%)	47 58
1	B	460/491 (94%)	439 (95%)	17 (4%)	4 (1%)	17 20
All	All	925/982 (94%)	889 (96%)	31 (3%)	5 (0%)	25 35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1394	LYS
1	B	1114	SER
1	B	1395	GLU
1	A	82	PRO
1	B	1404	ILE

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	410/440 (93%)	399 (97%)	11 (3%)	44 61
1	B	391/440 (89%)	377 (96%)	14 (4%)	35 49
All	All	801/880 (91%)	776 (97%)	25 (3%)	41 55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	118	LYS
1	A	195	LEU
1	A	277[A]	GLN
1	A	277[B]	GLN
1	A	314	PRO
1	A	336	LEU
1	A	421[A]	GLU
1	A	421[B]	GLU
1	A	423	ASN
1	B	1028	SER
1	B	1037	ASN
1	B	1123	ARG
1	B	1195	LEU
1	B	1262	PHE
1	B	1265	ASP
1	B	1314	PRO
1	B	1329	LEU
1	B	1394	LYS
1	B	1423	ASN
1	B	1424	GLU
1	B	1432	ASN
1	B	1460	GLU
1	B	1467	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	81	GLN
1	A	116	GLN
1	A	210	GLN
1	A	423	ASN
1	B	1020	GLN
1	B	1037	ASN
1	B	1258	ASN
1	B	1390	ASN
1	B	1423	ASN
1	B	1432	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are 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	SO4	B	503	-	4,4,4	0.75	0	6,6,6	0.39	0
2	SO4	A	505	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	B	501	-	4,4,4	0.27	0	6,6,6	0.20	0
2	SO4	B	506	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	A	504	-	4,4,4	0.45	0	6,6,6	0.06	0
2	SO4	B	502	-	4,4,4	0.26	0	6,6,6	0.15	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.