W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:24 PM GMT

PDB ID	:	5D3O
Title	:	Crystal structure of full length human glutaminase C expressed in E.coli
Authors	:	Huang, Q.
Deposited on	:	2015-08-06
Resolution	:	2.79 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982
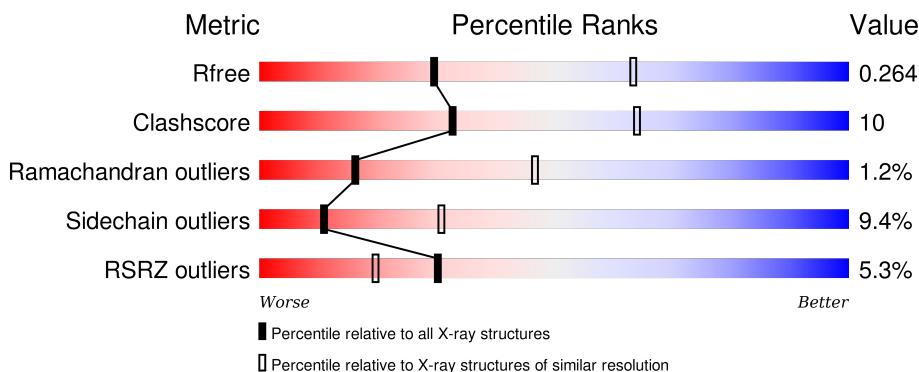
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
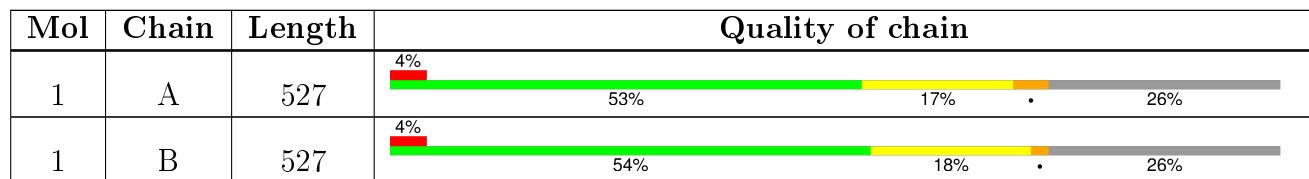
The reported resolution of this entry is 2.79 Å.

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	527	4% · 53% · 17% · 26%
1	B	527	4% · 54% · 18% · 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6082 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total 3052	C 1945	N 514	O 565	S 28	2	0	0
1	B	389	Total 3030	C 1933	N 510	O 559	S 28	2	0	0
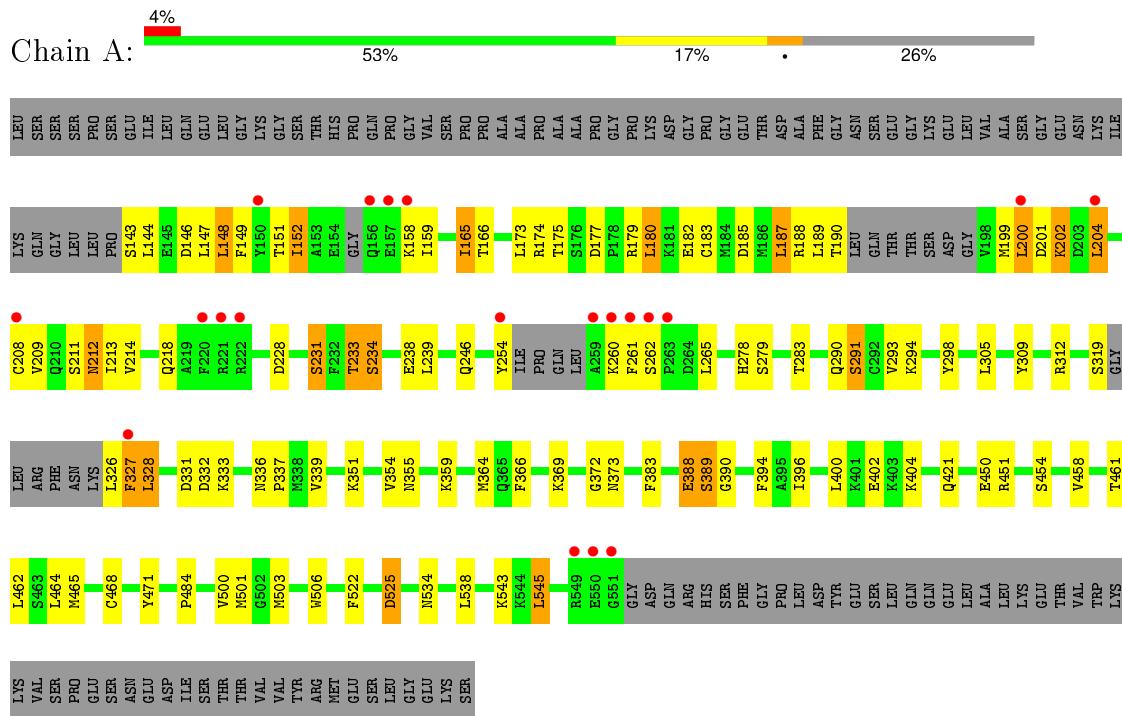
There are 2 discrepancies between the modelled and reference sequences:
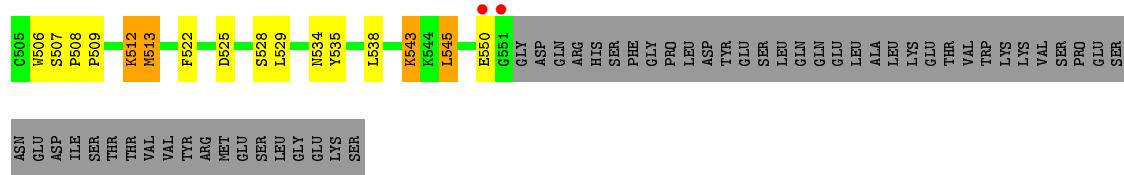
Chain	Residue	Modelled	Actual	Comment	Reference
A	273	ALA	VAL	conflict	UNP O94925
B	273	ALA	VAL	conflict	UNP O94925

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.

- Molecule 1: Glutaminase kidney isoform, mitochondrial

- Molecule 1: Glutaminase kidney isoform, mitochondrial

C505 W506 S507 P508 P509 K512 M513 F522 D525 S528 L529 N534 Y535 L538 K543 K544 L545 E550 G551 GLY ASP GLN ARG HIS SER PHE GLY PRO LEU ASP TYR GLU SER LEU GLN GLU LEU ALA LEU LYS GLU THR VAL TRP LYS LYS VAL SER PRO GLU SER

ASN GLU ASP ILE SER THR THR VAL VAL TYR ARG MET GLU SER LEU GLY GLU LYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.61Å 139.37Å 179.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.77 – 2.79 37.77 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.7 (37.77-2.79) 85.7 (37.77-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.214 , 0.266 0.208 , 0.264	Depositor DCC
R_{free} test set	1455 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 32826 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6082	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.46	0/3117	0.58	1/4200 (0.0%)
1	B	0.45	0/3095	0.56	0/4171
All	All	0.46	0/6212	0.57	1/8371 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	545	LEU	CA-CB-CG	5.45	127.83	115.30

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	3052	0	3013	63	0
1	B	3030	0	2993	63	0
All	All	6082	0	6006	125	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 10.

All (125) 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:145:GLU:HG3	1:B:206:LYS:HG3	1.54	0.89
1:A:228:ASP:OD2	1:A:231:SER:HB3	1.75	0.86
1:B:177:ASP:OD1	1:B:179:ARG:HD3	1.81	0.80
1:A:351:LYS:HB3	1:A:359:LYS:HG2	1.65	0.77
1:A:182:GLU:HG2	1:A:212:ASN:HD21	1.48	0.77
1:A:326:LEU:O	1:A:327:PHE:HB2	1.82	0.77
1:B:432:ALA:HA	1:B:435:MET:HG3	1.68	0.75
1:A:158:LYS:HB3	1:A:199:MET:HE3	1.72	0.71
1:A:461:THR:HG22	1:A:465:MET:HE2	1.72	0.71
1:B:512:LYS:HD2	1:B:513:MET:H	1.56	0.70
1:B:148:LEU:O	1:B:152:ILE:HG22	1.92	0.69
1:B:233:THR:HG23	1:B:278:HIS:CE1	2.29	0.68
1:A:148:LEU:O	1:A:152:ILE:HG22	1.93	0.68
1:B:529:LEU:HG	1:B:545:LEU:HD11	1.77	0.67
1:B:239:LEU:HD22	1:B:525:ASP:HB3	1.75	0.66
1:B:152:ILE:O	1:B:152:ILE:HG12	1.96	0.65
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.62	0.65
1:A:177:ASP:OD1	1:A:179:ARG:HD3	1.96	0.64
1:A:233:THR:HG23	1:A:278:HIS:CE1	2.33	0.63
1:B:503:MET:HE1	1:B:522:PHE:CE2	2.35	0.61
1:B:472:ASP:HB2	1:B:513:MET:HG2	1.83	0.60
1:A:158:LYS:HB3	1:A:199:MET:CE	2.32	0.60
1:B:186:MET:HG2	1:B:208:CYS:HA	1.84	0.58
1:A:503:MET:HE1	1:A:522:PHE:CE2	2.38	0.58
1:A:354:VAL:HG23	1:A:355:ASN:N	2.18	0.56
1:A:182:GLU:HG2	1:A:212:ASN:ND2	2.20	0.56
1:A:369:LYS:HG2	1:A:450:GLU:OE2	2.05	0.55
1:B:219:ALA:HB2	1:B:224:PHE:CZ	2.41	0.55
1:B:283:THR:HA	1:B:429:CYS:HB2	1.89	0.54
1:A:183:CYS:HB2	1:A:212:ASN:OD1	2.07	0.54
1:B:294:LYS:HD3	1:B:343:ALA:HB2	1.89	0.54
1:A:182:GLU:HG3	1:A:211:SER:HB2	1.88	0.54
1:A:200:LEU:HD12	1:A:204:LEU:HD13	1.90	0.53
1:A:461:THR:HG22	1:A:465:MET:CE	2.37	0.53
1:B:259:ALA:C	1:B:260:LYS:HD3	2.29	0.53
1:A:305:LEU:HD13	1:A:309:TYR:CE1	2.44	0.53
1:B:218:GLN:HG2	1:B:223:LYS:HB2	1.92	0.52
1:A:372:GLY:O	1:A:373:ASN:HB2	2.08	0.52
1:B:209:VAL:HG13	1:B:216:LEU:HD12	1.91	0.52
1:A:390:GLY:O	1:A:394:PHE:HD1	1.93	0.52
1:B:354:VAL:HG23	1:B:359:LYS:HG3	1.92	0.52
1:A:148:LEU:HD12	1:A:148:LEU:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ILE:O	1:B:152:ILE:CG1	2.58	0.50
1:A:503:MET:HE1	1:A:522:PHE:HE2	1.76	0.50
1:B:326:LEU:O	1:B:327:PHE:HB2	2.10	0.50
1:B:177:ASP:HB3	1:B:180:LEU:HB2	1.93	0.50
1:B:209:VAL:HG12	1:B:213:ILE:HD13	1.93	0.50
1:A:262:SER:HB3	1:A:265:LEU:HG	1.92	0.50
1:A:291:SER:CB	1:A:471:TYR:OH	2.60	0.50
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.93	0.50
1:A:214:VAL:HG12	1:A:218:GLN:NE2	2.26	0.50
1:A:454:SER:O	1:A:458:VAL:HG23	2.11	0.50
1:A:290:GLN:O	1:A:293:VAL:HG12	2.12	0.49
1:A:265:LEU:HD13	1:A:506:TRP:CH2	2.47	0.49
1:A:336:ASN:O	1:A:339:VAL:HG22	2.12	0.49
1:A:383:PHE:CE1	1:A:421:GLN:HG3	2.47	0.49
1:A:291:SER:HB3	1:A:294:LYS:NZ	2.29	0.48
1:B:454:SER:O	1:B:458:VAL:HG23	2.14	0.48
1:B:512:LYS:CD	1:B:513:MET:H	2.24	0.48
1:A:337:PRO:CG	1:A:464:LEU:HD13	2.44	0.48
1:A:149:PHE:CD1	1:A:159:ILE:HD11	2.49	0.47
1:B:291:SER:O	1:B:294:LYS:HG3	2.14	0.47
1:A:396:ILE:HG22	1:A:400:LEU:HD11	1.97	0.47
1:B:286:PRO:HA	1:B:427:VAL:O	2.15	0.47
1:B:364:MET:HE2	1:B:364:MET:HB3	1.65	0.47
1:B:314:VAL:HG22	1:B:315:GLY:N	2.30	0.46
1:A:149:PHE:CE1	1:A:159:ILE:HG13	2.50	0.46
1:A:484:PRO:HG3	1:B:535:TYR:CE2	2.50	0.46
1:A:336:ASN:HB2	1:A:337:PRO:HD2	1.97	0.46
1:A:234:SER:O	1:A:238:GLU:HG3	2.15	0.46
1:B:179:ARG:HD2	1:B:447:ILE:C	2.36	0.46
1:A:312:ARG:O	1:A:333:LYS:HE2	2.16	0.46
1:B:294:LYS:N	1:B:295:PRO:CD	2.79	0.45
1:B:508:PRO:HB2	1:B:509:PRO:HD3	1.98	0.45
1:B:289:LEU:O	1:B:292:CYS:HB2	2.16	0.45
1:A:500:VAL:HG12	1:A:501:MET:HB3	1.97	0.45
1:B:174:ARG:O	1:B:177:ASP:HB2	2.16	0.45
1:A:326:LEU:O	1:A:327:PHE:CB	2.60	0.45
1:B:179:ARG:HD2	1:B:447:ILE:O	2.17	0.45
1:B:385:SER:O	1:B:388:GLU:HB3	2.17	0.45
1:B:167:ALA:O	1:B:170:SER:HB3	2.17	0.44
1:A:501:MET:HE3	1:A:503:MET:SD	2.57	0.44
1:A:388:GLU:O	1:A:389:SER:HB3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:O	1:A:188:ARG:HG2	2.17	0.44
1:B:291:SER:HB3	1:B:294:LYS:NZ	2.32	0.44
1:A:279:SER:HB3	1:A:283:THR:HG21	1.98	0.44
1:B:437:ALA:HB1	1:B:446:PRO:HG3	1.99	0.44
1:B:200:LEU:CD1	1:B:204:LEU:HD22	2.49	0.43
1:B:260:LYS:C	1:B:261:PHE:HD1	2.22	0.43
1:A:188:ARG:C	1:A:190:THR:H	2.22	0.43
1:A:209:VAL:HG12	1:A:213:ILE:HD13	2.01	0.43
1:A:187:LEU:HD13	1:A:208:CYS:HB3	2.01	0.43
1:B:149:PHE:CE1	1:B:159:ILE:HD12	2.53	0.43
1:B:503:MET:HE1	1:B:522:PHE:HE2	1.80	0.43
1:A:147:LEU:O	1:A:151:THR:HG23	2.19	0.43
1:B:330:GLU:HA	1:B:330:GLU:OE2	2.18	0.43
1:A:396:ILE:HG22	1:A:400:LEU:CD1	2.49	0.42
1:B:529:LEU:HG	1:B:545:LEU:CD1	2.48	0.42
1:B:383:PHE:CE1	1:B:421:GLN:HG2	2.54	0.42
1:A:462:LEU:HD23	1:A:465:MET:HE1	2.01	0.42
1:A:298:TYR:CE2	1:A:464:LEU:HD12	2.55	0.42
1:B:543:LYS:HG2	1:B:543:LYS:H	1.67	0.42
1:B:209:VAL:CG1	1:B:213:ILE:HD13	2.49	0.42
1:A:165:ILE:HD12	1:A:165:ILE:HA	1.77	0.42
1:B:503:MET:HE3	1:B:503:MET:HB3	1.83	0.41
1:B:161:VAL:HG13	1:B:162:HIS:N	2.35	0.41
1:B:184:MET:O	1:B:188:ARG:HB2	2.20	0.41
1:A:143:SER:HB3	1:A:146:ASP:OD2	2.21	0.41
1:A:146:ASP:OD1	1:A:202:LYS:HE3	2.20	0.41
1:B:266:TRP:CE3	1:B:507:SER:HB2	2.55	0.41
1:B:185:ASP:HA	1:B:188:ARG:NH1	2.35	0.41
1:B:266:TRP:HA	1:B:506:TRP:O	2.19	0.41
1:A:328:LEU:HD13	1:A:332:ASP:O	2.20	0.41
1:B:176:SER:O	1:B:177:ASP:C	2.59	0.41
1:B:545:LEU:CD1	1:B:545:LEU:H	2.34	0.41
1:B:200:LEU:HD13	1:B:204:LEU:HD22	2.01	0.41
1:A:543:LYS:HD3	1:A:543:LYS:HA	1.72	0.41
1:B:305:LEU:HD13	1:B:309:TYR:CE1	2.55	0.41
1:B:498:PRO:O	1:B:499:ASN:HB2	2.21	0.41
1:A:328:LEU:HD13	1:A:332:ASP:C	2.40	0.41
1:A:351:LYS:O	1:A:359:LYS:HE2	2.21	0.41
1:B:331:ASP:N	1:B:331:ASP:OD1	2.54	0.41
1:B:483:LEU:HD22	1:B:497:VAL:HA	2.01	0.41
1:B:175:THR:HG22	1:B:176:SER:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.78	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	381/527 (72%)	353 (93%)	23 (6%)	5 (1%)	15	44
1	B	379/527 (72%)	343 (90%)	32 (8%)	4 (1%)	17	50
All	All	760/1054 (72%)	696 (92%)	55 (7%)	9 (1%)	16	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	SER
1	B	260	LYS
1	A	327	PHE
1	B	327	PHE
1	B	550	GLU
1	A	189	LEU
1	B	199	MET
1	A	202	LYS
1	A	246	GLN

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	337/451 (75%)	303 (90%)	34 (10%)	9	27
1	B	334/451 (74%)	305 (91%)	29 (9%)	13	35
All	All	671/902 (74%)	608 (91%)	63 (9%)	11	31

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	148	LEU
1	A	152	ILE
1	A	165	ILE
1	A	166	THR
1	A	173	LEU
1	A	174	ARG
1	A	175	THR
1	A	180	LEU
1	A	187	LEU
1	A	200	LEU
1	A	201	ASP
1	A	204	LEU
1	A	212	ASN
1	A	231	SER
1	A	233	THR
1	A	234	SER
1	A	254	TYR
1	A	260	LYS
1	A	261	PHE
1	A	291	SER
1	A	319	SER
1	A	328	LEU
1	A	331	ASP
1	A	364	MET
1	A	366	PHE
1	A	388	GLU
1	A	402	GLU
1	A	404	LYS
1	A	468	CYS
1	A	525	ASP
1	A	534	ASN
1	A	538	LEU
1	A	545	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ASP
1	B	147	LEU
1	B	173	LEU
1	B	175	THR
1	B	180	LEU
1	B	189	LEU
1	B	199	MET
1	B	203	ASP
1	B	204	LEU
1	B	207	LYS
1	B	217	THR
1	B	230	MET
1	B	233	THR
1	B	260	LYS
1	B	280	THR
1	B	326	LEU
1	B	331	ASP
1	B	365	GLN
1	B	366	PHE
1	B	386	GLU
1	B	493	ILE
1	B	504	MET
1	B	512	LYS
1	B	513	MET
1	B	528	SER
1	B	534	ASN
1	B	538	LEU
1	B	543	LYS
1	B	545	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	ASN
1	B	276	GLN
1	B	368	ASN
1	B	534	ASN

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)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	391/527 (74%)	0.32	20 (5%)	32	21	63, 81, 123, 142	2 (0%)
1	B	389/527 (73%)	0.28	21 (5%)	29	19	64, 81, 124, 160	2 (0%)
All	All	780/1054 (74%)	0.30	41 (5%)	30	20	63, 81, 124, 160	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	PHE	7.3
1	B	261	PHE	6.8
1	B	263	PRO	6.1
1	B	262	SER	5.1
1	B	150	TYR	4.3
1	A	204	LEU	4.3
1	B	147	LEU	4.1
1	B	551	GLY	4.1
1	A	221	ARG	4.0
1	A	263	PRO	4.0
1	A	262	SER	3.4
1	B	327	PHE	3.4
1	B	550	GLU	3.1
1	B	152	ILE	3.0
1	B	213	ILE	2.9
1	B	153	ALA	2.9
1	A	327	PHE	2.9
1	B	159	ILE	2.9
1	A	157	GLU	2.8
1	B	205	PHE	2.8
1	B	143	SER	2.8
1	A	551	GLY	2.8
1	B	260	LYS	2.7
1	A	259	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	2.7
1	A	254	TYR	2.6
1	B	158	LYS	2.6
1	A	222	ARG	2.4
1	B	218	GLN	2.4
1	A	156	GLN	2.3
1	A	260	LYS	2.2
1	A	158	LYS	2.2
1	B	200	LEU	2.2
1	A	150	TYR	2.2
1	A	220	PHE	2.2
1	B	328	LEU	2.1
1	A	549	ARG	2.1
1	B	151	THR	2.1
1	A	208	CYS	2.1
1	B	146	ASP	2.0
1	A	550	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.