



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:24 PM GMT

PDB ID : 1OWC
Title : Three Dimensional Structure Analysis Of The R109L Variant of the Type II Citrate Synthase From E. Coli
Authors : Stokell, D.J.; Donald, L.J.; Maurus, R.; Nguyen, N.T.; Sadler, G.; Choudhary, K.; Hultin, P.G.; Brayer, G.D.; Duckworth, H.W.
Deposited on : 2003-03-28
Resolution : 2.20 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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

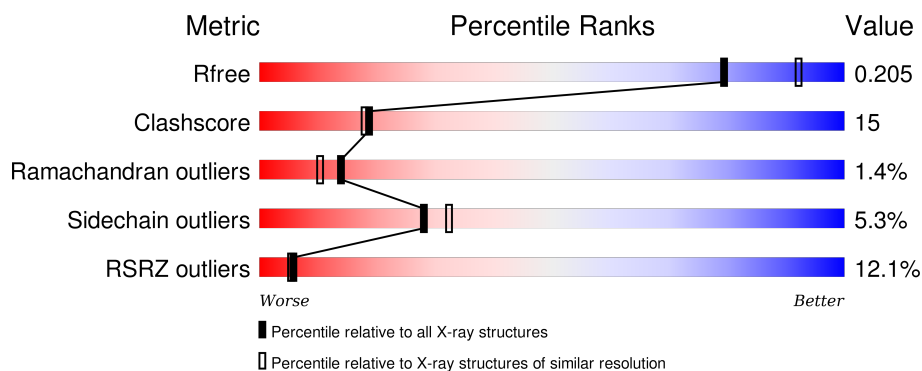
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div>12%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	B	427	<div> <div>12%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2002	-	X	-	-
2	SO4	B	2001	-	X	-	-
2	SO4	B	2003	-	X	-	-
2	SO4	B	2005	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7267 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.

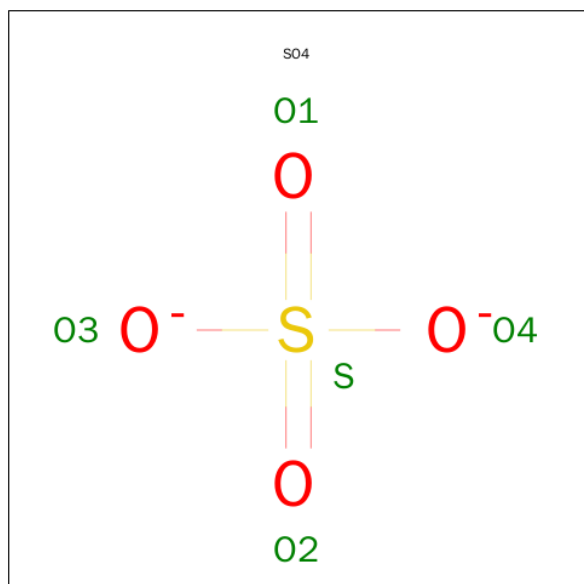
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3363	2135	576	627	25			
1	B	426	Total	C	N	O	S	0	0	0
			3363	2135	576	627	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	LEU	ARG	ENGINEERED	UNP P0ABH7
B	1109	LEU	ARG	ENGINEERED	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

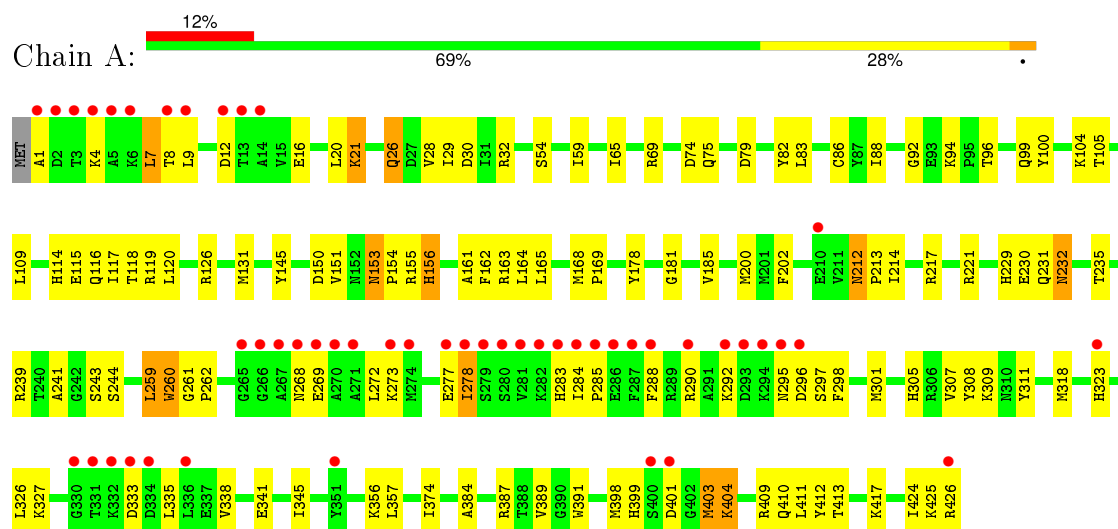
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total	O	0	0
			258	258		
3	B	253	Total	O	0	0
			253	253		

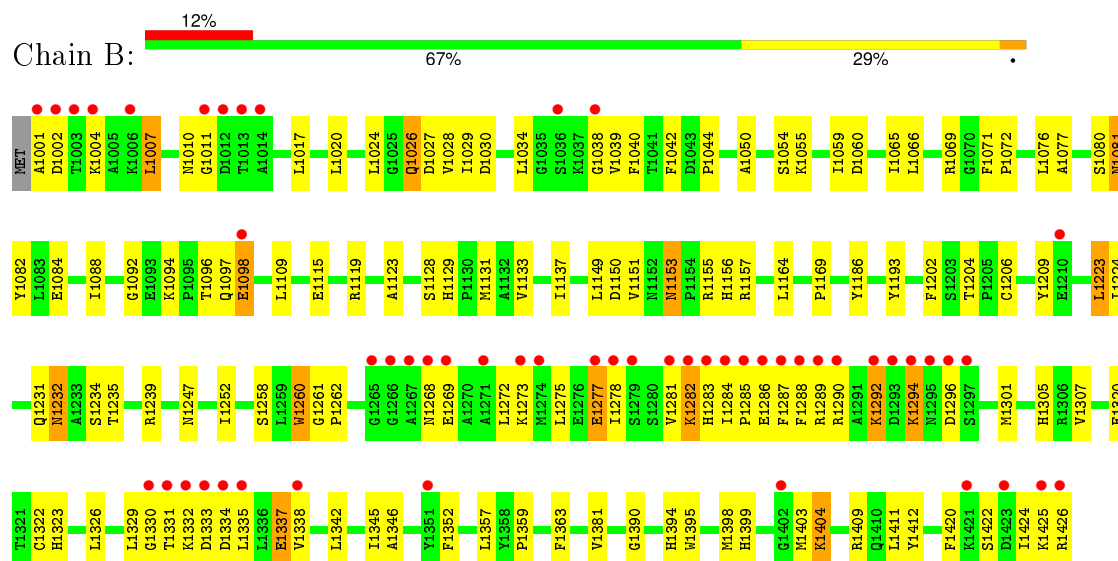
3 Residue-property plots [i](#)

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: Citrate synthase



• Molecule 1: Citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	165.07Å 165.07Å 155.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20 14.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 88.8 (14.86-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.24 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.161 , 0.210 0.172 , 0.205	Depositor DCC
R_{free} test set	2376 reflections (3.49%)	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.4	EDS
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71184 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7267	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.40	0/3441	0.64	0/4651
1	B	0.39	0/3441	0.62	0/4651
All	All	0.39	0/6882	0.63	0/9302

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	3363	0	3311	113	0
1	B	3363	0	3308	114	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	258	0	0	4	0
3	B	253	0	0	6	0
All	All	7267	0	6619	206	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 15.

All (206) 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:1290:ARG:HH12	1:B:1342:LEU:HA	1.09	1.07
1:B:1290:ARG:NH1	1:B:1342:LEU:HA	1.87	0.88
1:A:21:LYS:HE2	1:A:21:LYS:H	1.40	0.86
1:A:425:LYS:H	1:B:1097:GLN:HE22	1.19	0.86
1:B:1268:ASN:HD21	1:B:1296:ASP:HB2	1.41	0.84
1:A:305:HIS:HD2	1:A:307:VAL:H	1.27	0.81
1:B:1007:LEU:HD21	1:B:1029:ILE:HG23	1.61	0.81
1:A:1:ALA:HA	1:A:4:LYS:HD2	1.62	0.80
1:B:1186:TYR:HB3	3:B:399:HOH:O	1.83	0.79
1:B:1204:THR:HG22	1:B:1206:CYS:H	1.49	0.77
1:B:1020:LEU:HD23	1:B:1028:VAL:HG23	1.66	0.77
1:B:1425:LYS:HA	1:B:1425:LYS:HE2	1.67	0.77
1:B:1278:ILE:O	1:B:1284:ILE:HD11	1.88	0.74
1:A:284:ILE:HG21	1:A:338:VAL:HB	1.70	0.73
1:A:150:ASP:H	1:A:156:HIS:HD2	1.36	0.72
1:B:1153:ASN:HD22	1:B:1155:ARG:H	1.37	0.72
1:B:1115:GLU:HG3	1:B:1119:ARG:HH11	1.55	0.71
1:A:290:ARG:HG3	1:A:345:ILE:HG21	1.73	0.69
1:B:1305:HIS:HD2	1:B:1307:VAL:H	1.38	0.69
1:B:1269:GLU:HA	1:B:1272:LEU:HB2	1.75	0.69
1:B:1290:ARG:NE	1:B:1345:ILE:HD12	2.09	0.68
1:A:398:MET:SD	1:A:403:MET:HE1	2.34	0.67
1:A:296:ASP:HB2	1:A:298:PHE:HD2	1.59	0.67
1:B:1268:ASN:ND2	1:B:1296:ASP:HB2	2.09	0.67
1:B:1096:THR:HB	1:B:1098:GLU:HG3	1.79	0.65
1:A:21:LYS:H	1:A:21:LYS:CE	2.10	0.65
1:B:1335:LEU:HD23	1:B:1335:LEU:H	1.60	0.65
1:A:259:LEU:HD22	1:A:384:ALA:HB2	1.79	0.65
1:A:105:THR:O	1:A:109:LEU:HD23	1.95	0.64
1:A:425:LYS:N	1:B:1097:GLN:HE22	1.94	0.64
1:B:1001:ALA:HB1	1:B:1004:LYS:HB2	1.80	0.64
1:A:153:ASN:HD22	1:A:153:ASN:C	2.02	0.64
1:A:404:LYS:CD	1:A:404:LYS:H	2.11	0.63
1:B:1284:ILE:HB	1:B:1285:PRO:HD3	1.81	0.62
1:B:1284:ILE:HB	1:B:1285:PRO:CD	2.29	0.62
1:A:278:ILE:HG13	1:A:288:PHE:HE1	1.63	0.62
1:A:269:GLU:O	1:A:273:LYS:HD3	2.01	0.61
1:A:404:LYS:HD3	1:A:404:LYS:H	1.67	0.60
1:A:100:TYR:CE1	1:B:1426:ARG:HB3	2.36	0.60
1:A:9:LEU:HD11	1:B:1007:LEU:HD12	1.83	0.59
1:A:404:LYS:HG3	1:B:1044:PRO:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASP:OD1	1:A:32:ARG:HD3	2.02	0.59
1:A:278:ILE:HG22	1:A:284:ILE:HG13	1.83	0.59
1:A:398:MET:SD	1:A:403:MET:CE	2.91	0.58
1:B:1290:ARG:HH12	1:B:1342:LEU:CA	2.00	0.58
1:B:1088:ILE:HG12	1:B:1094:LYS:HA	1.86	0.58
1:A:100:TYR:HE1	1:B:1426:ARG:HB3	1.69	0.58
1:B:1077:ALA:HA	1:B:1224:ILE:HG21	1.86	0.57
1:B:1153:ASN:ND2	1:B:1155:ARG:H	2.02	0.57
1:A:296:ASP:HB2	1:A:298:PHE:CD2	2.38	0.57
1:B:1129:HIS:HD2	1:B:1131:MET:H	1.51	0.57
1:B:1115:GLU:HG3	1:B:1119:ARG:NH1	2.20	0.57
1:B:1278:ILE:HG21	1:B:1283:HIS:CG	2.40	0.57
1:A:268:ASN:HA	1:A:297:SER:OG	2.05	0.57
1:A:20:LEU:HB2	1:A:28:VAL:HG23	1.87	0.56
1:A:413:THR:HG22	3:A:2079:HOH:O	2.05	0.56
1:A:116:GLN:HE22	1:A:119:ARG:HE	1.53	0.56
1:A:131:MET:HE2	1:A:260:TRP:HB3	1.88	0.56
1:B:1281:VAL:HG23	1:B:1282:LYS:HD3	1.87	0.55
1:A:403:MET:HE3	1:A:403:MET:HA	1.89	0.55
1:B:1281:VAL:HG13	1:B:1338:VAL:HG12	1.89	0.55
1:A:86:CYS:HA	1:A:389:VAL:HG21	1.90	0.54
1:A:277:GLU:HG3	1:A:278:ILE:H	1.72	0.54
1:B:1020:LEU:O	1:B:1027:ASP:HB3	2.08	0.54
1:A:212:ASN:C	1:A:212:ASN:HD22	2.12	0.53
1:A:231:GLN:HE22	1:A:239:ARG:NE	2.07	0.53
1:B:1404:LYS:HE3	3:B:272:HOH:O	2.08	0.53
1:A:185:VAL:HB	1:A:200:MET:HA	1.91	0.53
1:B:1359:PRO:HB3	1:B:1363:PHE:CD2	2.43	0.53
1:B:1420:PHE:CZ	1:B:1422:SER:HB2	2.44	0.53
1:B:1096:THR:HG22	1:B:1097:GLN:H	1.73	0.52
1:A:231:GLN:HE22	1:A:239:ARG:HE	1.58	0.52
1:A:164:LEU:O	1:A:168:MET:HG2	2.08	0.52
1:A:7:LEU:HB2	1:B:1010:ASN:O	2.08	0.52
1:A:126:ARG:NH1	1:A:181:GLY:HA2	2.24	0.52
1:A:424:ILE:HA	1:B:1097:GLN:NE2	2.25	0.52
1:B:1150:ASP:H	1:B:1156:HIS:HD2	1.57	0.52
1:A:284:ILE:N	1:A:285:PRO:HD2	2.25	0.52
1:B:1322:CYS:O	1:B:1326:LEU:HD13	2.10	0.52
1:B:1149:LEU:HD22	1:B:1247:ASN:HB2	1.91	0.52
1:B:1153:ASN:HD22	1:B:1153:ASN:C	2.13	0.52
1:B:1169:PRO:HG3	1:B:1193:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:HD22	1:A:213:PRO:N	2.08	0.51
1:B:1081:ASN:ND2	1:B:1084:GLU:H	2.09	0.51
1:B:1026:GLN:HE21	1:B:1027:ASP:H	1.58	0.51
1:B:1151:VAL:HB	1:B:1399:HIS:CE1	2.46	0.51
1:A:284:ILE:CG2	1:A:338:VAL:HB	2.39	0.50
1:A:283:HIS:HB3	1:A:288:PHE:CD1	2.46	0.50
1:A:403:MET:HA	1:A:403:MET:CE	2.41	0.50
1:A:96:THR:H	1:A:99:GLN:HE21	1.60	0.50
1:B:1034:LEU:HD22	1:B:1039:VAL:HG11	1.94	0.50
1:A:323:HIS:CE1	1:A:327:LYS:HE3	2.47	0.50
1:B:1060:ASP:HB3	1:B:1065:ILE:HB	1.91	0.50
1:A:54:SER:O	1:B:1412:TYR:HA	2.12	0.50
1:A:202:PHE:HZ	1:A:374:ILE:HG13	1.77	0.49
1:B:1007:LEU:HD23	1:B:1017:LEU:O	2.13	0.49
1:B:1305:HIS:CD2	1:B:1307:VAL:H	2.26	0.49
1:A:153:ASN:ND2	1:A:155:ARG:H	2.09	0.49
1:A:404:LYS:HG3	1:B:1044:PRO:CB	2.42	0.49
1:A:217:ARG:O	1:A:221:ARG:HG3	2.11	0.49
1:A:145:TYR:HB3	1:A:163:ARG:NH2	2.26	0.49
1:B:1082:TYR:CD1	1:B:1223:LEU:HB3	2.48	0.49
1:A:335:LEU:HD23	1:A:335:LEU:H	1.78	0.49
1:B:1320:GLU:O	1:B:1323:HIS:HB3	2.12	0.49
1:A:212:ASN:ND2	1:A:214:ILE:H	2.11	0.49
1:A:243:SER:HA	1:A:403:MET:HE1	1.94	0.49
1:A:283:HIS:HB3	1:A:288:PHE:HB3	1.95	0.49
1:B:1329:LEU:O	1:B:1331:THR:N	2.45	0.49
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.43	0.49
1:A:126:ARG:HD2	1:A:178:TYR:CZ	2.48	0.48
1:A:285:PRO:CB	1:A:341:GLU:HG2	2.43	0.48
1:A:9:LEU:HD11	1:B:1007:LEU:CD1	2.42	0.48
1:A:28:VAL:HB	1:B:1042:PHE:HB2	1.95	0.48
1:A:83:LEU:CD2	1:A:104:LYS:HD2	2.44	0.48
1:B:1151:VAL:HG12	1:B:1395:TRP:HZ2	1.78	0.48
1:B:1076:LEU:O	1:B:1080:SER:HB3	2.14	0.48
1:B:1131:MET:HG2	1:B:1260:TRP:CG	2.49	0.48
1:A:278:ILE:HG13	1:A:288:PHE:CE1	2.47	0.47
1:B:1381:VAL:HG23	3:B:273:HOH:O	2.14	0.47
1:B:1285:PRO:HB3	1:B:1342:LEU:HD23	1.97	0.47
1:A:26:GLN:HG2	1:B:1038:GLY:O	2.14	0.47
1:A:232:ASN:C	1:A:232:ASN:HD22	2.17	0.47
1:B:1020:LEU:HD21	1:B:1030:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:MET:N	1:A:169:PRO:HD2	2.30	0.47
1:A:162:PHE:HB3	3:A:2094:HOH:O	2.14	0.47
1:B:1096:THR:HG22	1:B:1097:GLN:N	2.29	0.47
1:A:272:LEU:HD23	1:A:301:MET:HG2	1.95	0.47
1:A:261:GLY:N	1:A:262:PRO:HD2	2.30	0.47
1:A:69:ARG:HD2	1:A:92:GLY:HA2	1.95	0.47
1:B:1398:MET:SD	1:B:1403:MET:HA	2.54	0.47
1:A:83:LEU:HD22	1:A:104:LYS:HD2	1.95	0.47
1:A:151:VAL:HB	1:A:399:HIS:NE2	2.30	0.47
1:A:69:ARG:CD	1:A:92:GLY:HA2	2.45	0.46
1:A:7:LEU:HD21	1:A:29:ILE:CG1	2.45	0.46
1:A:1:ALA:HB1	1:A:4:LYS:HB2	1.97	0.46
1:B:1425:LYS:CE	1:B:1425:LYS:HA	2.43	0.46
1:B:1129:HIS:CD2	1:B:1131:MET:H	2.34	0.46
1:A:153:ASN:HD22	1:A:154:PRO:N	2.13	0.46
1:B:1059:ILE:HG12	1:B:1066:LEU:HD13	1.98	0.46
1:A:7:LEU:HD21	1:A:29:ILE:HG12	1.98	0.46
1:B:1239:ARG:HA	3:B:176:HOH:O	2.15	0.46
1:A:12:ASP:HB3	3:A:2231:HOH:O	2.16	0.46
1:A:8:THR:HG22	1:A:16:GLU:HA	1.99	0.46
1:B:1290:ARG:NH1	1:B:1342:LEU:HD23	2.30	0.45
1:B:1269:GLU:O	1:B:1273:LYS:HB2	2.15	0.45
1:A:262:PRO:O	1:A:268:ASN:HB2	2.15	0.45
1:B:1290:ARG:CZ	1:B:1345:ILE:HD12	2.46	0.45
1:B:1333:ASP:O	1:B:1335:LEU:N	2.48	0.45
1:B:1131:MET:HG2	1:B:1260:TRP:CD2	2.51	0.45
1:A:29:ILE:N	1:A:29:ILE:HD12	2.32	0.45
1:A:28:VAL:HG22	1:B:1411:LEU:HD13	1.99	0.44
1:B:1290:ARG:HE	1:B:1345:ILE:HD12	1.79	0.44
1:A:120:LEU:HD23	1:B:1123:ALA:HB3	1.99	0.44
1:A:116:GLN:HE22	1:A:119:ARG:NE	2.15	0.44
1:B:1292:LYS:HB2	1:B:1292:LYS:NZ	2.32	0.44
1:B:1331:THR:C	1:B:1332:LYS:HD3	2.38	0.44
1:A:413:THR:HB	1:B:1055:LYS:HZ3	1.83	0.44
1:A:83:LEU:HD21	1:A:104:LYS:HA	1.99	0.44
1:B:1286:GLU:HG2	1:B:1287:PHE:CD2	2.53	0.44
1:B:1294:LYS:HD2	1:B:1294:LYS:N	2.33	0.44
1:B:1157:ARG:HG2	1:B:1395:TRP:CH2	2.54	0.43
1:A:417:LYS:C	1:A:417:LYS:HD3	2.39	0.43
1:B:1202:PHE:HB2	1:B:1209:TYR:CZ	2.53	0.43
1:A:285:PRO:CA	1:A:341:GLU:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LYS:H	1:B:1097:GLN:NE2	1.99	0.43
1:A:232:ASN:ND2	1:A:235:THR:H	2.16	0.43
1:A:412:TYR:CD1	1:B:1024:LEU:HB2	2.54	0.43
1:A:161:ALA:O	1:A:165:LEU:HB2	2.18	0.43
1:A:59:ILE:HA	1:A:65:ILE:O	2.19	0.42
1:B:1272:LEU:HD23	1:B:1301:MET:SD	2.59	0.42
1:B:1273:LYS:O	1:B:1277:GLU:HG2	2.19	0.42
1:A:426:ARG:HD2	3:A:2152:HOH:O	2.20	0.42
1:A:126:ARG:HH11	1:A:181:GLY:HA2	1.84	0.42
1:B:1034:LEU:HD22	1:B:1039:VAL:CG1	2.50	0.42
1:A:241:ALA:O	1:A:244:SER:HB2	2.18	0.42
1:A:32:ARG:HD2	1:B:1042:PHE:CD1	2.54	0.42
1:A:309:LYS:HZ3	1:A:356:LYS:HE3	1.84	0.42
1:B:1133:VAL:O	1:B:1137:ILE:HG12	2.19	0.42
1:A:308:TYR:HB3	1:A:311:TYR:O	2.19	0.42
1:A:115:GLU:O	1:A:118:THR:HB	2.19	0.42
1:A:82:TYR:CE2	1:A:86:CYS:SG	3.13	0.42
1:B:1153:ASN:ND2	1:B:1155:ARG:HB3	2.35	0.41
1:B:1234:SER:HA	1:B:1258:SER:OG	2.20	0.41
1:A:409:ARG:HB2	1:B:1050:ALA:HA	2.02	0.41
1:A:410:GLN:OE1	1:B:1054:SER:HB3	2.20	0.41
1:B:1071:PHE:HA	1:B:1072:PRO:HD3	1.91	0.41
1:B:1026:GLN:HA	1:B:1026:GLN:HE21	1.86	0.41
1:A:335:LEU:CD2	1:A:335:LEU:H	2.33	0.41
1:B:1128:SER:HA	3:B:84:HOH:O	2.21	0.41
1:A:387:ARG:HG3	1:A:391:TRP:CE2	2.55	0.41
1:A:285:PRO:HA	1:A:341:GLU:HG2	2.01	0.41
1:B:1150:ASP:OD1	1:B:1153:ASN:HB2	2.20	0.41
1:A:69:ARG:HG3	1:A:88:ILE:O	2.21	0.41
1:B:1069:ARG:HD2	1:B:1092:GLY:HA2	2.02	0.41
1:B:1283:HIS:N	3:B:165:HOH:O	2.54	0.41
1:B:1289:ARG:NH1	1:B:1290:ARG:HD3	2.36	0.41
1:B:1390:GLY:O	1:B:1394:HIS:HD2	2.03	0.41
1:B:1232:ASN:ND2	1:B:1235:THR:H	2.19	0.41
1:B:1164:LEU:HD13	1:B:1252:ILE:HG13	2.03	0.41
1:B:1352:PHE:HA	1:B:1357:LEU:HD12	2.02	0.41
1:A:114:HIS:HB3	1:A:117:ILE:HG13	2.03	0.41
1:B:1346:ALA:HA	1:B:1352:PHE:CD2	2.56	0.40
1:A:75:GLN:O	1:A:79:ASP:HB2	2.20	0.40
1:B:1040:PHE:CZ	1:B:1409:ARG:HD2	2.56	0.40
1:A:243:SER:HA	1:A:403:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1273:LYS:HB2	1:B:1273:LYS:HE2	1.92	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	424/427 (99%)	391 (92%)	31 (7%)	2 (0%)	34	35
1	B	424/427 (99%)	383 (90%)	31 (7%)	10 (2%)	7	4
All	All	848/854 (99%)	774 (91%)	62 (7%)	12 (1%)	14	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ILE
1	B	1330	GLY
1	B	1334	ASP
1	A	401	ASP
1	B	1002	ASP
1	B	1231	GLN
1	B	1261	GLY
1	B	1277	GLU
1	B	1337	GLU
1	B	1262	PRO
1	B	1011	GLY
1	B	1424	ILE

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	361/362 (100%)	339 (94%)	22 (6%)	23	26
1	B	361/362 (100%)	345 (96%)	16 (4%)	35	42
All	All	722/724 (100%)	684 (95%)	38 (5%)	28	32

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	21	LYS
1	A	26	GLN
1	A	74	ASP
1	A	94	LYS
1	A	153	ASN
1	A	156	HIS
1	A	212	ASN
1	A	229	HIS
1	A	230	GLU
1	A	232	ASN
1	A	259	LEU
1	A	260	TRP
1	A	292	LYS
1	A	295	ASN
1	A	318	MET
1	A	326	LEU
1	A	333	ASP
1	A	357	LEU
1	A	403	MET
1	A	404	LYS
1	A	411	LEU
1	B	1007	LEU
1	B	1026	GLN
1	B	1081	ASN
1	B	1098	GLU
1	B	1109	LEU

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Mol	Chain	Res	Type
1	B	1153	ASN
1	B	1223	LEU
1	B	1232	ASN
1	B	1260	TRP
1	B	1275	LEU
1	B	1282	LYS
1	B	1288	PHE
1	B	1292	LYS
1	B	1294	LYS
1	B	1337	GLU
1	B	1404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	99	GLN
1	A	116	GLN
1	A	153	ASN
1	A	156	HIS
1	A	182	GLN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	268	ASN
1	A	295	ASN
1	A	305	HIS
1	A	323	HIS
1	A	344	ASN
1	A	348	ASN
1	B	1026	GLN
1	B	1081	ASN
1	B	1097	GLN
1	B	1129	HIS
1	B	1153	ASN
1	B	1156	HIS
1	B	1232	ASN
1	B	1268	ASN
1	B	1305	HIS
1	B	1399	HIS

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 ⓘ

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	A	2002	-	4,4,4	1.09	0	6,6,6	3.63	4 (66%)
2	SO4	A	2004	-	4,4,4	0.82	0	6,6,6	0.19	0
2	SO4	A	2006	-	4,4,4	0.95	0	6,6,6	0.32	0
2	SO4	B	2001	-	4,4,4	0.96	0	6,6,6	3.63	4 (66%)
2	SO4	B	2003	-	4,4,4	0.83	0	6,6,6	3.62	4 (66%)
2	SO4	B	2005	-	4,4,4	1.10	0	6,6,6	3.64	4 (66%)

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	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2006	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2005	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2003	SO4	O4-S-O3	-5.76	85.55	108.98
2	A	2002	SO4	O4-S-O3	-5.66	85.97	108.98
2	B	2001	SO4	O4-S-O3	-5.64	86.04	108.98
2	B	2005	SO4	O4-S-O3	-5.30	87.44	108.98
2	B	2005	SO4	O4-S-O1	-3.51	77.55	110.19
2	B	2003	SO4	O4-S-O1	-3.27	79.78	110.19
2	A	2002	SO4	O4-S-O1	-3.20	80.44	110.19
2	B	2001	SO4	O4-S-O1	-3.16	80.80	110.19
2	B	2001	SO4	O4-S-O2	-2.72	84.86	110.19
2	A	2002	SO4	O4-S-O2	-2.66	85.46	110.19
2	B	2005	SO4	O4-S-O2	-2.57	86.25	110.19
2	B	2003	SO4	O4-S-O2	-2.56	86.34	110.19
2	B	2003	SO4	O2-S-O1	5.24	126.09	109.50
2	A	2002	SO4	O2-S-O1	5.39	126.58	109.50
2	B	2001	SO4	O2-S-O1	5.40	126.61	109.50
2	B	2005	SO4	O2-S-O1	5.65	127.40	109.50

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

6.1 Protein, DNA and RNA chains

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	426/427 (99%)	0.46	50 (11%) 6 6	8, 20, 62, 84	0
1	B	426/427 (99%)	0.39	53 (12%) 5 5	7, 19, 55, 78	0
All	All	852/854 (99%)	0.43	103 (12%) 6 5	7, 19, 59, 84	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	PRO	15.3
1	A	1	ALA	11.2
1	A	3	THR	11.1
1	A	287	PHE	8.5
1	A	331	THR	8.4
1	A	286	GLU	8.1
1	B	1002	ASP	8.0
1	B	1003	THR	7.8
1	A	4	LYS	7.5
1	A	332	LYS	7.3
1	A	295	ASN	7.2
1	B	1013	THR	6.5
1	B	1331	THR	6.5
1	A	283	HIS	6.4
1	B	1287	PHE	6.4
1	A	13	THR	6.3
1	A	2	ASP	6.3
1	B	1267	ALA	6.2
1	B	1288	PHE	6.2
1	B	1426	ARG	6.1
1	A	334	ASP	6.1
1	B	1284	ILE	6.0
1	B	1423	ASP	5.9
1	A	267	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	281	VAL	5.7
1	B	1278	ILE	5.5
1	B	1277	GLU	5.4
1	A	269	GLU	5.3
1	B	1001	ALA	5.3
1	B	1012	ASP	5.3
1	B	1332	LYS	5.3
1	A	265	GLY	5.2
1	A	290	ARG	5.2
1	B	1279	SER	5.1
1	B	1297	SER	4.9
1	B	1285	PRO	4.8
1	A	296	ASP	4.5
1	A	330	GLY	4.5
1	B	1286	GLU	4.4
1	B	1036	SER	4.4
1	B	1004	LYS	4.2
1	A	426	ARG	4.2
1	B	1295	ASN	4.1
1	A	288	PHE	4.1
1	A	282	LYS	4.1
1	B	1273	LYS	4.0
1	A	274	MET	4.0
1	A	292	LYS	3.9
1	A	284	ILE	3.9
1	B	1333	ASP	3.8
1	B	1334	ASP	3.7
1	A	12	ASP	3.7
1	B	1335	LEU	3.7
1	B	1265	GLY	3.6
1	B	1296	ASP	3.6
1	A	266	GLY	3.6
1	B	1283	HIS	3.5
1	A	280	SER	3.5
1	B	1294	LYS	3.5
1	B	1290	ARG	3.4
1	B	1271	ALA	3.4
1	B	1330	GLY	3.3
1	A	5	ALA	3.3
1	A	279	SER	3.3
1	A	293	ASP	3.3
1	B	1038	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1282	LYS	3.2
1	A	294	LYS	3.1
1	B	1266	GLY	3.1
1	B	1269	GLU	3.1
1	A	278	ILE	3.0
1	B	1425	LYS	3.0
1	A	277	GLU	3.0
1	A	8	THR	3.0
1	B	1338	VAL	2.9
1	B	1011	GLY	2.9
1	A	400	SER	2.9
1	B	1293	ASP	2.9
1	B	1274	MET	2.8
1	B	1210	GLU	2.8
1	A	14	ALA	2.8
1	B	1014	ALA	2.8
1	A	273	LYS	2.7
1	A	268	ASN	2.6
1	B	1268	ASN	2.6
1	A	9	LEU	2.6
1	A	336	LEU	2.5
1	B	1402	GLY	2.5
1	A	323	HIS	2.5
1	B	1421	LYS	2.5
1	B	1281	VAL	2.5
1	B	1351	TYR	2.4
1	A	271	ALA	2.3
1	A	6	LYS	2.3
1	B	1098	GLU	2.3
1	A	401	ASP	2.3
1	A	270	ALA	2.2
1	B	1006	LYS	2.2
1	B	1292	LYS	2.1
1	B	1289	ARG	2.1
1	A	210	GLU	2.0
1	A	333	ASP	2.0
1	A	351	TYR	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	2003	5/5	0.96	0.15	1.16	26,27,28,28	0
2	SO4	B	2001	5/5	0.98	0.09	-1.16	19,19,20,20	0
2	SO4	A	2006	5/5	0.99	0.07	-1.34	15,16,16,18	0
2	SO4	A	2004	5/5	0.99	0.08	-3.42	17,17,18,18	0
2	SO4	B	2005	5/5	0.85	0.20	-	39,39,40,40	0
2	SO4	A	2002	5/5	0.96	0.15	-	17,18,20,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.