



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:55 AM UTC

PDB ID : 1OWC / pdb_00001owc
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

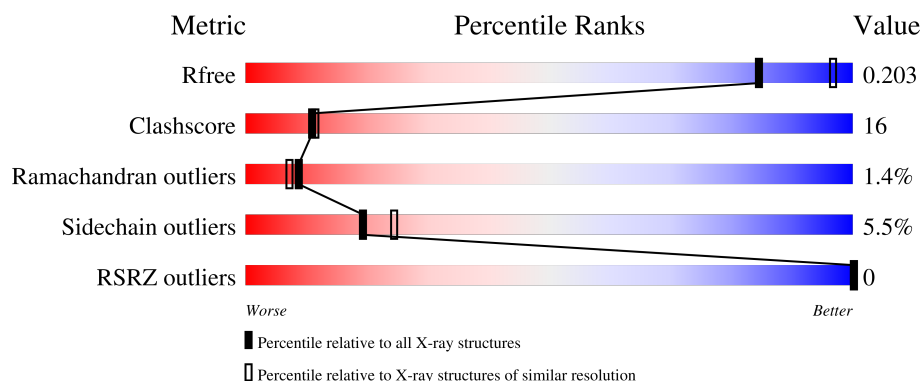
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	 66% 30% .
1	B	427	 65% 30% .

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.

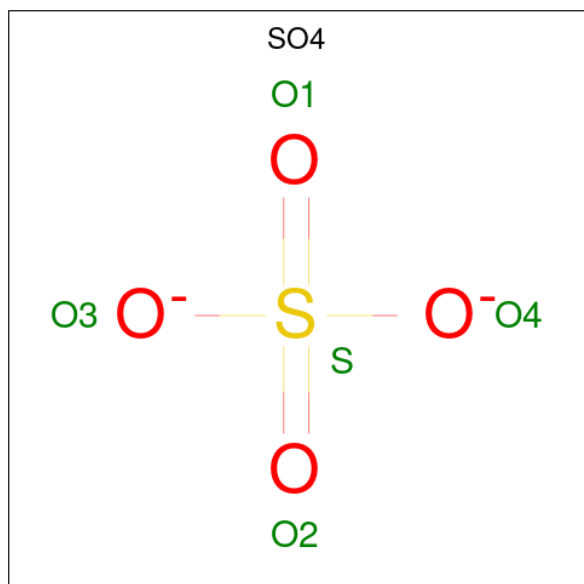
- Molecule 1 is a protein called Citrate synthase.

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 mutation	UNP P0ABH7
B	1109	LEU	ARG	engineered mutation	UNP P0ABH7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

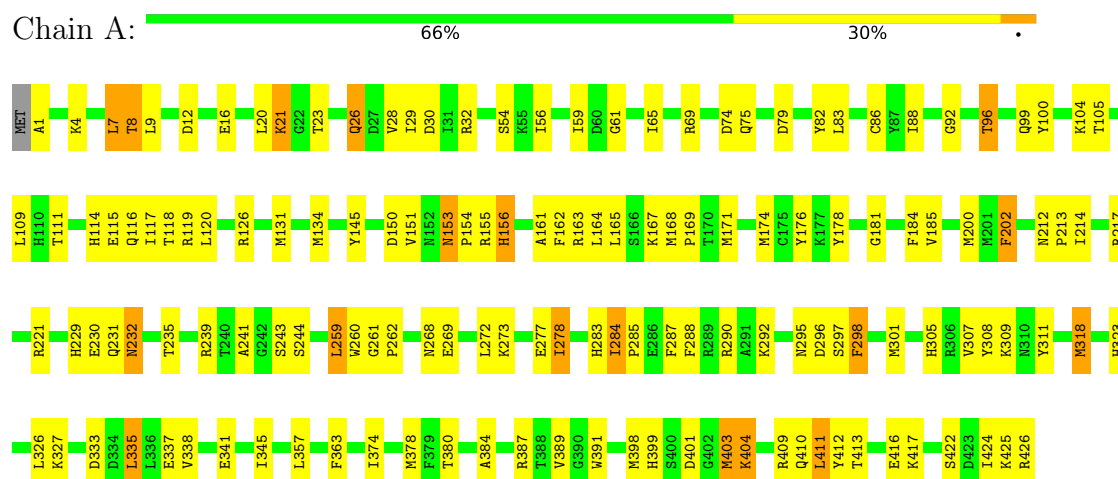
- Molecule 3 is water.

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

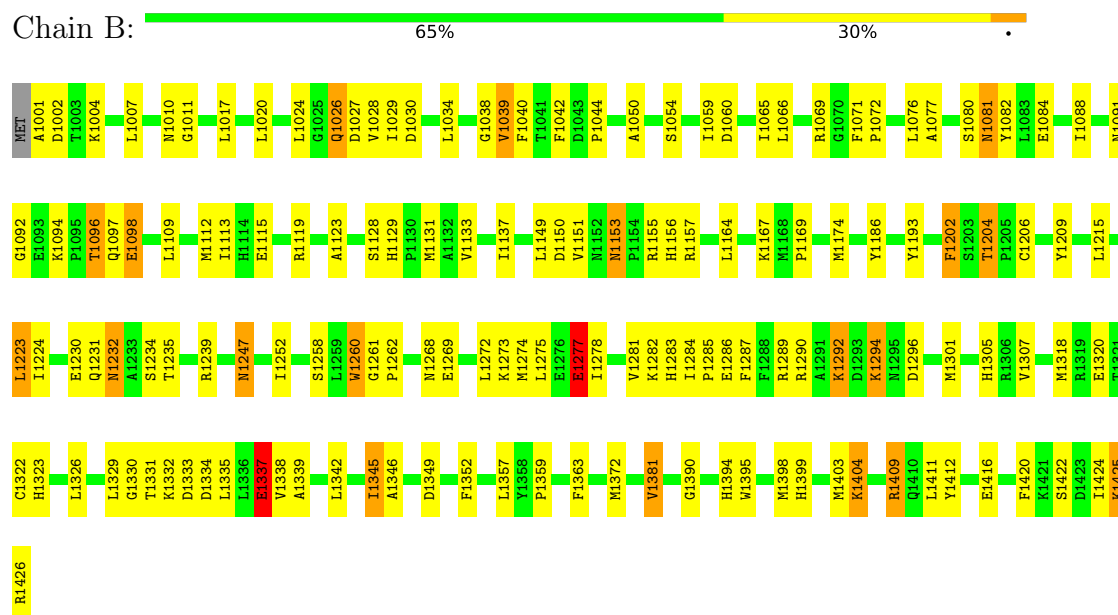
3 Residue-property plots

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 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 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 88.9 (10.00-2.20)	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 (Not available) , 0.203	Depositor DCC
R_{free} test set	2376 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.48	0/3441	1.04	16/4651 (0.3%)
1	B	0.47	0/3441	0.98	11/4651 (0.2%)
All	All	0.47	0/6882	1.01	27/9302 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ILE	N-CA-C	8.92	118.81	110.42
1	A	337	GLU	N-CA-C	-7.86	103.83	113.50
1	A	202	PHE	N-CA-C	7.67	123.79	113.97
1	A	287	PHE	N-CA-C	7.29	121.45	111.54
1	B	1096	THR	N-CA-C	-7.10	99.36	110.36
1	A	167	LYS	N-CA-C	7.06	121.65	112.89
1	A	309	LYS	N-CA-C	6.99	118.79	111.03
1	A	96	THR	N-CA-C	-6.81	101.54	110.53
1	B	1349	ASP	CA-C-N	6.50	126.26	119.05
1	B	1349	ASP	C-N-CA	6.50	126.26	119.05
1	A	363	PHE	N-CA-C	-6.38	104.25	111.14
1	B	1416	GLU	N-CA-C	-6.25	101.72	110.35
1	B	1202	PHE	N-CA-C	6.25	121.84	113.72
1	A	416	GLU	N-CA-C	-6.13	102.28	110.55
1	A	111	THR	N-CA-C	6.12	118.03	111.36
1	A	23	THR	N-CA-C	-6.07	105.71	113.23
1	B	1167	LYS	N-CA-C	6.04	120.38	112.89
1	A	422	SER	N-CA-C	5.82	117.81	110.24
1	B	1277	GLU	N-CA-C	5.82	123.19	110.80
1	B	1091	ASN	N-CA-C	5.76	120.37	113.23
1	A	8	THR	N-CA-C	5.43	117.65	109.23
1	A	298	PHE	N-CA-C	5.22	118.11	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLY	N-CA-C	5.21	118.98	112.73
1	A	411	LEU	N-CA-C	-5.13	100.15	108.41
1	B	1247	ASN	CA-C-N	5.07	124.51	119.24
1	B	1247	ASN	C-N-CA	5.07	124.51	119.24
1	B	1381	VAL	N-CA-C	-5.05	105.57	110.42

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	3363	0	3311	118	0
1	B	3363	0	3308	122	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	220	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 16.

All (220) 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:A:243:SER:HA	1:A:403:MET:HE1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:B:1425:LYS:HA	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:134:MET:HE1	1:A:171:MET:HB3	1.73	0.70
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:A:153:ASN:HD22	1:A:153:ASN:C	2.02	0.68
1:B:1290:ARG:NE	1:B:1345:ILE:HD12	2.09	0.68
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:H	1:B:1335:LEU:HD23	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:B:1318:MET:HE3	1:B:1318:MET:HA	1.80	0.63
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:A:278:ILE:HG13	1:A:288:PHE:HE1	1.63	0.62
1:B:1284:ILE:HB	1:B:1285:PRO:CD	2.29	0.62
1:A:134:MET:HE1	1:A:171:MET:CB	2.30	0.61
1:A:269:GLU:O	1:A:273:LYS:HD3	2.01	0.61
1:A:404:LYS:H	1:A:404:LYS:HD3	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:30:ASP:OD1	1:A:32:ARG:HD3	2.02	0.59
1:A:404:LYS:HG3	1:B:1044:PRO:HB3	1.83	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:HE3	2.43	0.58
1:B:1112:MET:HE2	1:B:1186:TYR:CD1	2.37	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:C	1:A:212:ASN:HD22	2.12	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:A:296:ASP:HB2	1:A:298:PHE:CD2	2.38	0.57
1:B:1153:ASN:ND2	1:B:1155:ARG:H	2.02	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:A:268:ASN:HA	1:A:297:SER:OG	2.05	0.57
1:B:1278:ILE:HG21	1:B:1283:HIS:CG	2.40	0.57
1:A:20:LEU:HB2	1:A:28:VAL:HG23	1.87	0.56
1:B:1153:ASN:HD22	1:B:1153:ASN:C	2.13	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:B:1281:VAL:HG23	1:B:1282:LYS:HD3	1.87	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: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:A:403:MET:HE2	1:A:403:MET:HA	1.90	0.53
1:B:1420:PHE:CZ	1:B:1422:SER:HB2	2.44	0.53
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:164:LEU:O	1:A:168:MET:HG2	2.08	0.52
1:A:231:GLN:HE22	1:A:239:ARG:HE	1.58	0.52
1:B:1096:THR:HG22	1:B:1097:GLN:H	1.73	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:A:131:MET:HE2	1:A:260:TRP:HB3	1.92	0.52
1:A:232:ASN:C	1:A:232:ASN:HD22	2.17	0.52
1:B:1149:LEU:HD22	1:B:1247:ASN:HB2	1.91	0.52
1:B:1322:CYS:O	1:B:1326:LEU:HD13	2.10	0.52
1:B:1169:PRO:HG3	1:B:1193:TYR:OH	2.10	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:A:403:MET:HA	2.41	0.50
1:A:96:THR:H	1:A:99:GLN:HE21	1.60	0.50
1:A:323:HIS:CE1	1:A:327:LYS:HE3	2.47	0.50
1:B:1034:LEU:HD22	1:B:1039:VAL:HG11	1.94	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:174:MET:HE3	1:A:184:PHE:CD2	2.47	0.50
1:A:202:PHE:HZ	1:A:374:ILE:HG13	1.77	0.49
1:A:145:TYR:HB3	1:A:163:ARG:NH2	2.26	0.49
1:A:153:ASN:ND2	1:A:155:ARG:H	2.09	0.49
1:A:217:ARG:O	1:A:221:ARG:HG3	2.11	0.49
1:A:404:LYS:HG3	1:B:1044:PRO:CB	2.42	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: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: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:B:1331:THR:C	1:B:1332:LYS:HD3	2.38	0.49
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.43	0.49
1:B:1215:LEU:HB3	1:B:1372:MET:HE3	1.95	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:A:417:LYS:HD3	1:A:417:LYS:C	2.39	0.48
1:A:398:MET:HE3	1:A:398:MET:HB3	1.78	0.48
1:B:1076:LEU:O	1:B:1080:SER:HB3	2.14	0.48
1:B:1151:VAL:HG12	1:B:1395:TRP:HZ2	1.78	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:A:26:GLN:HG2	1:B:1038:GLY:O	2.14	0.47
1:B:1285:PRO:HB3	1:B:1342:LEU:HD23	1.97	0.47
1:A:162:PHE:HB3	3:A:2094:HOH:O	2.14	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:B:1020:LEU:HD21	1:B:1030:ASP:HB2	1.96	0.47
1:A:272:LEU:HD23	1:A:301:MET:HG2	1.95	0.47
1:B:1096:THR:HG22	1:B:1097:GLN:N	2.29	0.47
1:A:69:ARG:HD2	1:A:92:GLY:HA2	1.95	0.47
1:A:261:GLY:N	1:A:262:PRO:HD2	2.30	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:1129:HIS:CD2	1:B:1131:MET:H	2.34	0.46
1:B:1425:LYS:HA	1:B:1425:LYS:CE	2.43	0.46
1:A:153:ASN:HD22	1:A:154:PRO:N	2.13	0.46
1:A:176:TYR:HB2	1:A:378:MET:HE2	1.98	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:A:8:THR:HG22	1:A:16:GLU:HA	1.99	0.46
1:A:12:ASP:HB3	3:A:2231:HOH:O	2.16	0.46
1:B:1239:ARG:HA	3:B:176:HOH:O	2.15	0.46
1:B:1290:ARG:NH1	1:B:1342:LEU:HD23	2.30	0.45
1:A:262:PRO:O	1:A:268:ASN:HB2	2.15	0.45
1:B:1269:GLU:O	1:B:1273:LYS: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:A:29:ILE:HD12	1:A:29:ILE:N	2.32	0.45
1:B:1131:MET:HG2	1:B:1260:TRP:CD2	2.51	0.45
1:A:28:VAL:HG22	1:B:1411:LEU:HD13	1.99	0.44
1:B:1081:ASN:C	1:B:1081:ASN:HD22	2.24	0.44
1:A:120:LEU:HD23	1:B:1123:ALA:HB3	1.99	0.44
1:B:1290:ARG:HE	1:B:1345:ILE:HD12	1.79	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: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:1081:ASN:ND2	1:B:1081:ASN:C	2.75	0.44
1:B:1294:LYS:HD2	1:B:1294:LYS:N	2.33	0.44
1:A:318:MET:HA	1:A:318:MET:HE3	2.00	0.43
1:B:1157:ARG:HG2	1:B:1395:TRP:CH2	2.54	0.43
1:B:1202:PHE:HB2	1:B:1209:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:CA	1:A:341:GLU:HG2	2.48	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:425:LYS:H	1:B:1097:GLN:NE2	1.99	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:1289:ARG:HH21	1:B:1301:MET:HE3	1.84	0.42
1:A:426:ARG:HD2	3:A:2152:HOH:O	2.20	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:126:ARG:HH11	1:A:181:GLY:HA2	1.84	0.42
1:A:241:ALA:O	1:A:244:SER:HB2	2.18	0.42
1:A:398:MET:SD	1:A:403:MET:HE1	2.58	0.42
1:B:1034:LEU:HD22	1:B:1039:VAL:CG1	2.50	0.42
1:B:1113:ILE:HD11	1:B:1174:MET:HE1	2.01	0.42
1:A:32:ARG:HD2	1:B:1042:PHE:CD1	2.54	0.42
1:B:1337:GLU:C	1:B:1339:ALA:H	2.26	0.42
1:B:1133:VAL:O	1:B:1137:ILE:HG12	2.19	0.42
1:A:115:GLU:O	1:A:118:THR:HB	2.19	0.42
1:A:308:TYR:HB3	1:A:311:TYR:O	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:131:MET:HE2	1:A:380:THR:HB	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:HE21	1:B:1026:GLN:HA	1.86	0.41
1:A:335:LEU:H	1:A:335:LEU:CD2	2.33	0.41
1:A:387:ARG:HG3	1:A:391:TRP:CE2	2.55	0.41
1:B:1128:SER:HA	3:B:84:HOH:O	2.21	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:B:1274:MET:HE1	1:B:1292:LYS:HG2	2.03	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:1164:LEU:HD13	1:B:1252:ILE:HG13	2.03	0.41
1:B:1232:ASN:ND2	1:B:1235:THR:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:HB3	1:A:117:ILE:HG13	2.03	0.41
1:B:1352:PHE:HA	1:B:1357:LEU:HD12	2.02	0.41
1:A:75:GLN:O	1:A:79:ASP:HB2	2.20	0.40
1:B:1346:ALA:HA	1:B:1352:PHE:CD2	2.56	0.40
1:B:1040:PHE:CZ	1:B:1409:ARG:HD2	2.56	0.40
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%)	24	27
1	B	424/427 (99%)	383 (90%)	31 (7%)	10 (2%)	4	3
All	All	848/854 (99%)	774 (91%)	62 (7%)	12 (1%)	9	7

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%)	340 (94%)	21 (6%)	18	22
1	B	361/362 (100%)	342 (95%)	19 (5%)	20	26
All	All	722/724 (100%)	682 (94%)	40 (6%)	19	24

All (40) 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	153	ASN
1	A	156	HIS
1	A	229	HIS
1	A	230	GLU
1	A	232	ASN
1	A	259	LEU
1	A	284	ILE
1	A	292	LYS
1	A	295	ASN
1	A	318	MET
1	A	326	LEU
1	A	333	ASP
1	A	335	LEU
1	A	357	LEU
1	A	403	MET
1	A	404	LYS
1	A	411	LEU
1	B	1026	GLN
1	B	1039	VAL
1	B	1081	ASN
1	B	1098	GLU
1	B	1109	LEU
1	B	1153	ASN

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Mol	Chain	Res	Type
1	B	1204	THR
1	B	1223	LEU
1	B	1230	GLU
1	B	1232	ASN
1	B	1260	TRP
1	B	1275	LEU
1	B	1292	LYS
1	B	1294	LYS
1	B	1337	GLU
1	B	1345	ILE
1	B	1404	LYS
1	B	1409	ARG
1	B	1425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	348	ASN
1	B	1026	GLN
1	B	1081	ASN
1	B	1097	GLN
1	B	1129	HIS
1	B	1152	ASN
1	B	1153	ASN
1	B	1156	HIS
1	B	1232	ASN
1	B	1305	HIS
1	B	1310	ASN
1	B	1344	ASN

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Mol	Chain	Res	Type
1	B	1348	ASN
1	B	1399	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2005	-	4,4,4	0.70	0	6,6,6	3.66	4 (66%)
2	SO4	A	2002	-	4,4,4	0.69	0	6,6,6	3.59	4 (66%)
2	SO4	B	2001	-	4,4,4	0.61	0	6,6,6	3.60	4 (66%)
2	SO4	A	2006	-	4,4,4	0.71	0	6,6,6	0.49	0
2	SO4	A	2004	-	4,4,4	0.66	0	6,6,6	0.28	0
2	SO4	B	2003	-	4,4,4	0.56	0	6,6,6	3.60	4 (66%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2005	SO4	O4-S-O1	-6.12	77.55	109.56
2	B	2003	SO4	O4-S-O1	-5.70	79.78	109.56
2	A	2002	SO4	O4-S-O1	-5.57	80.44	109.56
2	B	2001	SO4	O4-S-O1	-5.50	80.80	109.56
2	B	2001	SO4	O4-S-O2	-4.73	84.86	109.56
2	A	2002	SO4	O4-S-O2	-4.61	85.46	109.56
2	B	2005	SO4	O4-S-O2	-4.46	86.25	109.56
2	B	2003	SO4	O4-S-O2	-4.44	86.34	109.56
2	B	2003	SO4	O4-S-O3	-4.17	85.55	108.54
2	A	2002	SO4	O4-S-O3	-4.09	85.97	108.54
2	B	2001	SO4	O4-S-O3	-4.08	86.04	108.54
2	B	2005	SO4	O4-S-O3	-3.83	87.44	108.54
2	B	2005	SO4	O2-S-O1	2.60	127.40	109.06
2	B	2001	SO4	O2-S-O1	2.49	126.61	109.06
2	A	2002	SO4	O2-S-O1	2.49	126.58	109.06
2	B	2003	SO4	O2-S-O1	2.42	126.09	109.06

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](#)

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%)	-1.74	0 100 100	8, 20, 62, 84	0
1	B	426/427 (99%)	-1.75	0 100 100	7, 19, 55, 78	0
All	All	852/854 (99%)	-1.74	0 100 100	7, 19, 59, 84	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
2	SO4	A	2002	5/5	1.00	0.02	17,18,20,21	0
2	SO4	A	2004	5/5	1.00	0.01	17,17,18,18	0
2	SO4	A	2006	5/5	1.00	0.01	15,16,16,18	0
2	SO4	B	2001	5/5	1.00	0.01	19,19,20,20	0
2	SO4	B	2003	5/5	1.00	0.01	26,27,28,28	0
2	SO4	B	2005	5/5	1.00	0.02	39,39,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.