WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:41 PM GMT

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PDB ID	:	1LI7
Title	:	Crystal Structure of Cysteinyl-tRNA Synthetase with Cysteine Substrate Bound
Authors	:	Newberry, K.J.; Hou, Y.-M.; Perona, J.J.
Deposited on	:	2002-04-17
Resolution	:	2.60 Å(reported)

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	461	
1	B	461	

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
3	CYS	B	1001	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5827 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.
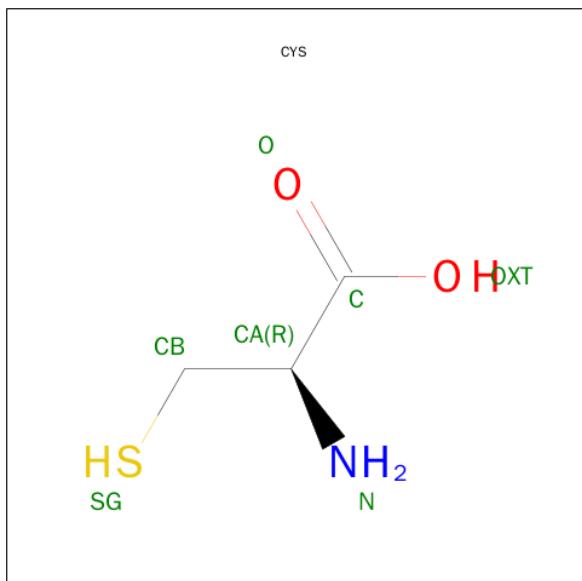
- Molecule 1 is a protein called CYSTEINYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2961	1874	513	549	25			
1	B	375	Total	C	N	O	S	0	0	0
			2779	1763	484	510	22			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
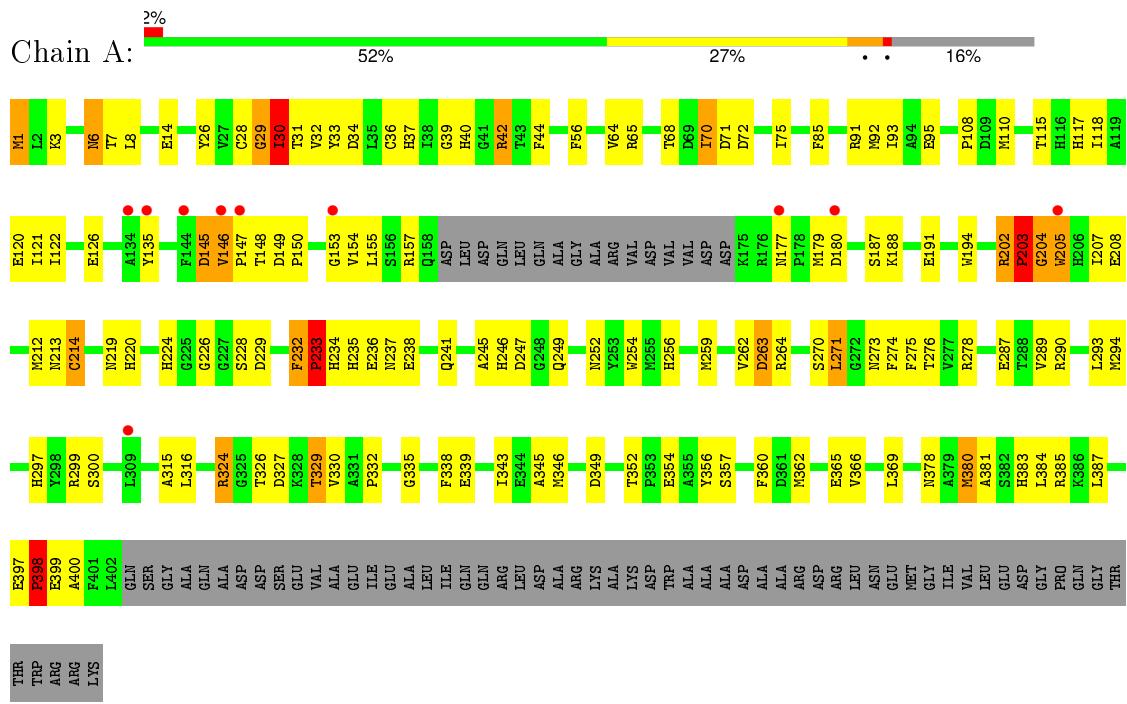
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	33	Total	O	0	0
			33	33		
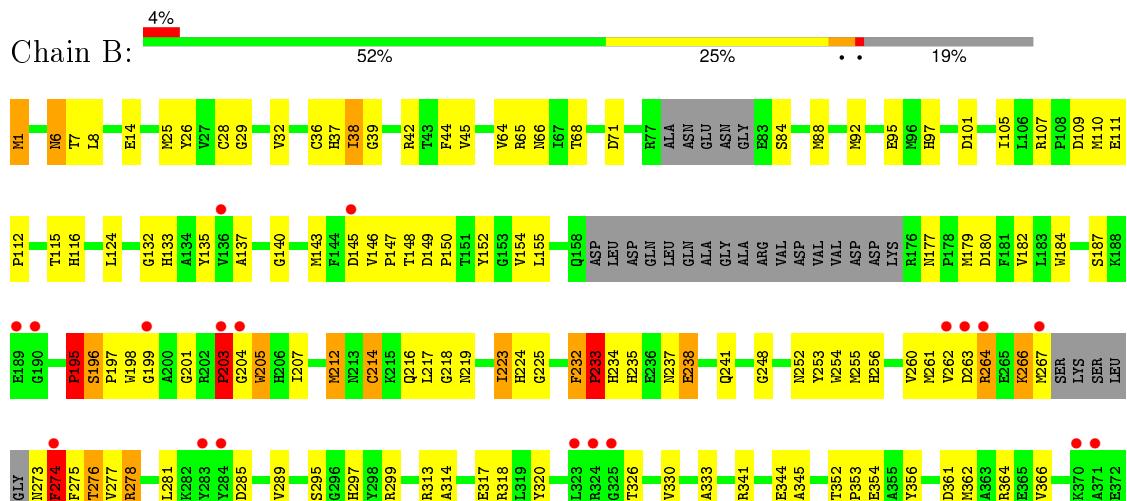
3 Residue-property plots ⓘ
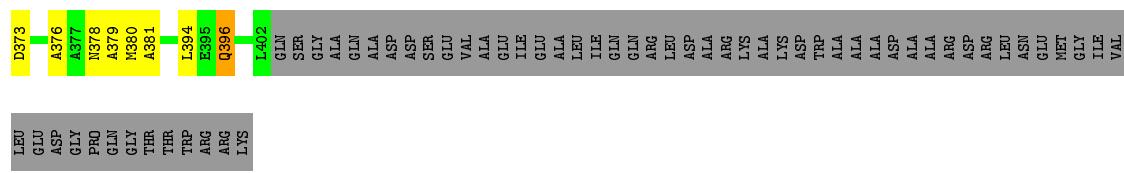
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: CYSTEINYL-TRNA SYNTHETASE

- Molecule 1: CYSTEINYL-TRNA SYNTHETASE

D373 A376 A377 N378 A379 M380 A381 L394 E395 Q396 L402 GLN SER GLY ALA GLN ALA ASP ASP SER GLU VAL ALA GLU ILE GLU ALA LEU ILE GLN GLN ARG LEU ASP ALA ARG LYS ALA LYS ASP TRP ALA ALA ALA ASP ALA ALA ARG ASP ARG LEU ASN GLU MET GLY ILE VAL

LEU GLU ASP GLY PRO GLN GLY THR THR TRP ARG ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.98Å　　118.98Å　　143.84Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	19.95　–　2.60 54.97　–　2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-2.60) 100.0 (54.97-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.35 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250　,　0.290 0.249　,　0.289	Depositor DCC
R_{free} test set	3222 reflections (9.97%)	DCC
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 32397 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

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

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	3/3033 (0.1%)	0.94	14/4117 (0.3%)
1	B	0.49	1/2846 (0.0%)	0.80	7/3874 (0.2%)
All	All	0.51	4/5879 (0.1%)	0.88	21/7991 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CD-OE2	-9.34	1.15	1.25
1	A	30	ILE	N-CA	-6.20	1.33	1.46
1	A	29	GLY	CA-C	-5.25	1.43	1.51
1	A	29	GLY	N-CA	-5.03	1.38	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	PHE	C-N-CD	-20.14	76.29	120.60
1	A	233	PRO	CA-N-CD	-19.03	84.86	111.50
1	A	232	PHE	C-N-CD	-17.51	82.07	120.60
1	B	232	PHE	C-N-CA	13.74	179.70	122.00
1	A	398	PRO	CA-N-CD	-11.70	95.12	111.50
1	A	233	PRO	CA-CB-CG	-10.28	84.47	104.00
1	A	232	PHE	C-N-CA	9.65	162.55	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	HIS	CB-CA-C	-9.04	92.31	110.40
1	A	203	PRO	CA-N-CD	-8.64	99.40	111.50
1	B	203	PRO	CA-N-CD	-7.64	100.81	111.50
1	A	29	GLY	C-N-CA	-6.27	106.01	121.70
1	A	246	HIS	CA-C-N	-6.13	103.71	117.20
1	A	246	HIS	N-CA-CB	6.13	121.63	110.60
1	A	233	PRO	N-CD-CG	6.06	112.28	103.20
1	A	233	PRO	N-CA-CB	5.80	110.26	103.30
1	B	233	PRO	CA-N-CD	-5.72	103.49	111.50
1	B	248	GLY	C-N-CA	-5.62	107.64	121.70
1	A	247	ASP	CA-C-N	-5.45	105.30	116.20
1	B	260	VAL	CB-CA-C	-5.38	101.18	111.40
1	B	274	PHE	CA-CB-CG	-5.30	101.18	113.90
1	A	233	PRO	CB-CG-CD	-5.11	86.59	106.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	88	MET	Mainchain

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	2961	0	2743	123	0
1	B	2779	0	2485	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	7	0	3	3	0
3	B	7	0	3	5	0
4	A	38	0	0	1	0
4	B	33	0	0	0	0
All	All	5827	0	5234	242	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 22.

All (242) 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:68:THR:HG1	3:B:1001:CYS:N	1.58	1.00
1:A:287:GLU:HG2	1:A:316:LEU:HD21	1.44	0.97
1:B:149:ASP:HB3	1:B:152:TYR:HB2	1.51	0.93
1:A:146:VAL:HG22	1:A:147:PRO:HD3	1.53	0.89
1:B:38:ILE:HD12	1:B:39:GLY:H	1.40	0.86
1:B:333:ALA:HB3	1:B:379:ALA:HB1	1.58	0.86
1:B:205:TRP:HE1	3:B:1001:CYS:HA	1.41	0.84
1:B:148:THR:O	1:B:150:PRO:HD3	1.76	0.84
1:A:362:MET:HE3	1:A:384:LEU:HD13	1.58	0.84
1:B:330:VAL:HG21	1:B:378:ASN:HB3	1.59	0.84
1:A:235:HIS:HD2	1:A:256:HIS:HE1	1.24	0.83
1:A:235:HIS:HD2	1:A:256:HIS:CE1	1.99	0.81
1:A:68:THR:HG1	3:A:1000:CYS:N	1.80	0.80
1:B:112:PRO:HB2	1:B:212:MET:HG2	1.64	0.80
1:A:37:HIS:HA	1:A:276:THR:HA	1.63	0.79
1:A:324:ARG:HG2	1:A:324:ARG:NH1	1.99	0.76
1:B:232:PHE:CD2	1:B:233:PRO:HD3	2.20	0.76
1:A:346:MET:HE3	1:A:352:THR:HA	1.66	0.75
1:A:324:ARG:HG2	1:A:324:ARG:HH11	1.48	0.75
1:B:275:PHE:O	1:B:276:THR:CB	2.35	0.75
1:B:235:HIS:HD2	1:B:256:HIS:NE2	1.84	0.74
1:B:320:TYR:OH	1:B:396:GLN:HG3	1.87	0.74
1:A:65:ARG:HH11	1:A:65:ARG:HG2	1.54	0.73
1:A:229:ASP:H	1:A:259:MET:HE3	1.54	0.73
1:A:26:TYR:CD1	1:A:213:ASN:HB3	2.25	0.72
1:B:101:ASP:OD1	1:B:107:ARG:NH1	2.23	0.71
1:B:143:MET:CE	1:B:182:VAL:HG22	2.21	0.71
1:B:237:ASN:O	1:B:241:GLN:HG3	1.92	0.69
1:A:70:ILE:HG23	1:A:85:PHE:CE1	2.28	0.69
1:B:263:ASP:O	1:B:264:ARG:CB	2.41	0.69
1:A:232:PHE:CD2	1:A:233:PRO:HD3	2.28	0.68
1:A:117:HIS:O	1:A:121:ILE:HG13	1.93	0.68
1:A:204:GLY:O	1:A:205:TRP:CB	2.40	0.68
1:B:6:ASN:HD21	1:B:8:LEU:HB2	1.57	0.68
1:B:135:TYR:HE1	1:B:137:ALA:HB2	1.58	0.68
1:B:143:MET:HE2	1:B:182:VAL:HA	1.75	0.68
1:B:143:MET:HE1	1:B:182:VAL:HG22	1.74	0.67
1:B:262:VAL:H	1:B:266:LYS:CB	2.07	0.67
1:B:326:THR:HG21	1:B:381:ALA:CB	2.25	0.67
1:A:324:ARG:HH11	1:A:324:ARG:CG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:MET:HE1	1:A:384:LEU:HA	1.77	0.67
1:A:262:VAL:HB	1:A:273:ASN:HB2	1.75	0.67
1:B:223:ILE:HD13	1:B:255:MET:SD	2.35	0.67
1:B:132:GLY:O	1:B:148:THR:HG21	1.95	0.67
1:B:37:HIS:HA	1:B:276:THR:HA	1.77	0.66
1:B:146:VAL:HB	1:B:147:PRO:HD3	1.78	0.66
1:B:204:GLY:O	1:B:207:ILE:HG22	1.95	0.66
1:B:326:THR:HG21	1:B:381:ALA:HB3	1.78	0.65
1:B:66:ASN:HB2	1:B:212:MET:CE	2.26	0.65
1:A:31:THR:HA	1:A:68:THR:HB	1.79	0.65
1:B:154:VAL:HG13	1:B:155:LEU:N	2.12	0.65
1:B:124:LEU:HD22	1:B:207:ILE:HD11	1.76	0.65
1:B:313:ARG:O	1:B:317:GLU:HG3	1.97	0.65
1:A:220:HIS:HE1	1:A:252:ASN:OD1	1.80	0.65
1:A:32:VAL:HG22	1:A:92:MET:HB3	1.78	0.64
1:A:7:THR:OG1	1:A:256:HIS:HD2	1.80	0.64
1:B:6:ASN:ND2	1:B:8:LEU:H	1.96	0.63
1:B:133:HIS:ND1	1:B:148:THR:CG2	2.61	0.63
1:A:145:ASP:HA	1:A:180:ASP:OD1	1.98	0.63
1:A:326:THR:HG21	1:A:381:ALA:CB	2.29	0.62
1:A:226:GLY:O	1:A:256:HIS:HA	1.98	0.62
1:B:196:SER:C	1:B:198:TRP:H	2.03	0.62
1:B:101:ASP:CG	1:B:107:ARG:HH12	2.03	0.62
1:B:6:ASN:ND2	1:B:8:LEU:HB2	2.14	0.62
1:A:28:CYS:SG	1:A:235:HIS:HE1	2.24	0.60
1:B:65:ARG:HG2	1:B:65:ARG:HH11	1.67	0.60
1:A:1:MET:HG3	1:A:14:GLU:HG3	1.82	0.60
1:B:361:ASP:HA	1:B:364:ARG:NH1	2.17	0.60
1:A:30:ILE:HD11	1:A:40:HIS:CG	2.37	0.59
1:B:95:GLU:CD	1:B:278:ARG:HH21	2.05	0.59
1:B:320:TYR:CZ	1:B:394:LEU:HA	2.37	0.59
1:A:95:GLU:HG3	1:A:278:ARG:NH2	2.17	0.59
1:B:38:ILE:HD12	1:B:39:GLY:N	2.15	0.59
1:A:32:VAL:HG13	1:A:32:VAL:O	2.03	0.59
1:B:277:VAL:HG23	1:B:278:ARG:N	2.18	0.59
1:B:184:TRP:HE1	1:B:201:GLY:HA3	1.66	0.59
1:A:72:ASP:OD2	1:A:202:ARG:NH2	2.34	0.59
1:A:37:HIS:HD2	1:A:39:GLY:H	1.49	0.58
1:B:184:TRP:NE1	1:B:201:GLY:HA3	2.17	0.58
1:B:184:TRP:CZ3	1:B:203:PRO:HD3	2.38	0.58
1:A:369:LEU:CD1	1:A:380:MET:HG3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:VAL:O	1:A:263:ASP:CB	2.51	0.58
1:B:133:HIS:O	1:B:145:ASP:N	2.28	0.57
1:A:95:GLU:HG3	1:A:278:ARG:HH22	1.68	0.57
1:A:224:HIS:HE1	1:A:238:GLU:OE1	1.87	0.57
1:A:70:ILE:HG23	1:A:85:PHE:CZ	2.39	0.57
1:A:339:GLU:OE1	1:A:383:HIS:HE1	1.87	0.57
1:A:369:LEU:HD12	1:A:380:MET:HG3	1.86	0.57
1:B:133:HIS:ND1	1:B:148:THR:HG21	2.19	0.57
1:A:362:MET:HE3	1:A:384:LEU:CD1	2.34	0.57
1:A:335:GLY:H	1:A:383:HIS:CD2	2.21	0.57
1:A:297:HIS:HE1	1:A:349:ASP:O	1.88	0.56
1:A:121:ILE:HG23	1:A:207:ILE:HG13	1.86	0.56
1:B:97:HIS:HE1	1:B:111:GLU:OE1	1.88	0.56
1:A:65:ARG:HB3	1:A:108:PRO:HG2	1.88	0.56
1:A:235:HIS:CD2	1:A:256:HIS:HE1	2.15	0.56
1:A:28:CYS:HB3	3:A:1000:CYS:SG	2.45	0.56
1:B:205:TRP:NE1	3:B:1001:CYS:HA	2.15	0.56
1:B:29:GLY:HA3	1:B:66:ASN:O	2.06	0.56
1:A:315:ALA:HB1	1:A:360:PHE:HZ	1.71	0.56
1:A:146:VAL:CG2	1:A:147:PRO:HD3	2.33	0.55
1:A:326:THR:CG2	1:A:385:ARG:HH22	2.18	0.55
1:B:92:MET:O	1:B:95:GLU:N	2.39	0.55
1:A:335:GLY:H	1:A:383:HIS:HD2	1.54	0.55
1:A:366:VAL:HG22	1:A:380:MET:HB3	1.89	0.54
1:B:266:LYS:O	1:B:267:MET:C	2.45	0.54
1:B:273:ASN:O	1:B:274:PHE:CB	2.54	0.54
1:A:362:MET:CE	1:A:384:LEU:HA	2.38	0.54
1:A:204:GLY:O	1:A:205:TRP:HB3	2.07	0.54
1:A:65:ARG:NH1	1:A:65:ARG:HG2	2.20	0.54
1:B:214:CYS:HB2	1:B:219:ASN:HD22	1.73	0.54
1:A:290:ARG:HG2	1:A:294:MET:CE	2.38	0.53
1:B:261:MET:HG2	1:B:267:MET:C	2.29	0.53
1:B:225:GLY:HA2	1:B:255:MET:O	2.08	0.53
1:B:66:ASN:HB2	1:B:212:MET:HE1	1.90	0.53
1:A:362:MET:CE	1:A:387:LEU:HD12	2.38	0.53
1:A:135:TYR:CE2	1:A:145:ASP:HB3	2.44	0.53
1:B:195:PRO:O	1:B:196:SER:CB	2.57	0.52
1:B:109:ASP:O	1:B:110:MET:HG2	2.09	0.52
1:A:338:PHE:HE1	1:A:380:MET:HE3	1.75	0.52
1:B:285:ASP:O	1:B:289:VAL:HG23	2.10	0.52
1:A:188:LYS:O	1:A:191:GLU:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:CYS:HB3	3:B:1001:CYS:HB3	1.91	0.51
1:A:153:GLY:O	1:A:157:ARG:N	2.43	0.51
1:B:6:ASN:C	1:B:6:ASN:HD22	2.13	0.51
1:B:38:ILE:CD1	1:B:39:GLY:H	2.19	0.51
1:A:365:GLU:HG2	1:A:380:MET:HE3	1.93	0.51
1:A:115:THR:O	1:A:118:ILE:HD12	2.10	0.51
1:B:341:ARG:NH2	1:B:361:ASP:OD2	2.44	0.50
1:B:64:VAL:HG23	1:B:217:LEU:HD21	1.93	0.50
1:B:330:VAL:HG21	1:B:378:ASN:CB	2.37	0.50
1:A:327:ASP:OD1	1:A:329:THR:HG22	2.11	0.50
1:A:270:SER:OG	1:A:271:LEU:HD13	2.11	0.50
1:B:112:PRO:CB	1:B:212:MET:HG2	2.40	0.50
1:B:318:ARG:HH11	1:B:318:ARG:HG3	1.75	0.50
1:B:318:ARG:HG3	1:B:318:ARG:NH1	2.26	0.50
1:A:177:ASN:ND2	1:A:179:MET:HB2	2.27	0.50
1:B:66:ASN:HB2	1:B:212:MET:HE3	1.93	0.50
1:A:346:MET:HA	1:A:346:MET:CE	2.41	0.49
1:B:124:LEU:HD22	1:B:207:ILE:CD1	2.42	0.49
1:A:42:ARG:NH2	1:A:300:SER:O	2.44	0.49
1:B:154:VAL:CG1	1:B:155:LEU:N	2.76	0.49
1:A:146:VAL:HG21	1:A:179:MET:HE3	1.95	0.49
1:B:177:ASN:ND2	1:B:179:MET:H	2.11	0.49
1:B:362:MET:O	1:B:366:VAL:HG23	2.13	0.49
1:A:32:VAL:HG22	1:A:92:MET:CB	2.41	0.49
1:B:224:HIS:HE1	1:B:238:GLU:OE1	1.96	0.49
1:B:187:SER:H	1:B:201:GLY:HA2	1.78	0.48
1:B:110:MET:HE2	1:B:110:MET:HA	1.94	0.48
1:A:235:HIS:CD2	1:A:256:HIS:CE1	2.91	0.48
1:B:330:VAL:CG2	1:B:378:ASN:HB3	2.37	0.48
1:A:30:ILE:HD13	1:A:36:CYS:HB3	1.96	0.47
1:A:214:CYS:HB2	1:A:219:ASN:HD22	1.79	0.47
1:B:262:VAL:C	1:B:264:ARG:H	2.17	0.47
1:B:133:HIS:CE1	1:B:148:THR:HG22	2.49	0.47
1:A:32:VAL:HG21	1:A:93:ILE:HG13	1.96	0.47
1:A:290:ARG:HG2	1:A:294:MET:HE2	1.96	0.47
1:A:26:TYR:HA	1:A:64:VAL:O	2.15	0.47
1:A:121:ILE:HG23	1:A:207:ILE:CG1	2.44	0.47
1:B:36:CYS:O	1:B:277:VAL:HG22	2.15	0.47
1:A:29:GLY:HA2	1:A:44:PHE:CZ	2.49	0.47
1:A:148:THR:O	1:A:150:PRO:HD3	2.14	0.47
1:B:297:HIS:HD2	1:B:299:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG12	1:A:68:THR:O	2.15	0.47
1:A:326:THR:HG21	1:A:381:ALA:HB3	1.97	0.47
1:B:352:THR:OG1	1:B:353:PRO:HD3	2.15	0.46
1:A:154:VAL:HG13	1:A:155:LEU:N	2.30	0.46
1:B:45:VAL:HG23	1:B:105:ILE:HD11	1.97	0.46
1:A:71:ASP:OD2	1:A:71:ASP:O	2.33	0.46
1:A:362:MET:HE1	1:A:387:LEU:HD12	1.97	0.46
1:A:6:ASN:HD22	1:A:6:ASN:C	2.17	0.46
1:A:399:GLU:O	1:A:400:ALA:C	2.53	0.46
1:A:115:THR:HG23	1:A:194:TRP:HZ2	1.81	0.46
1:B:146:VAL:HG23	1:B:180:ASP:HA	1.97	0.46
1:A:274:PHE:CD2	1:A:274:PHE:C	2.88	0.46
1:B:235:HIS:CD2	1:B:256:HIS:NE2	2.75	0.46
1:B:107:ARG:HG2	1:B:107:ARG:HH11	1.81	0.46
1:B:6:ASN:HD22	1:B:7:THR:N	2.13	0.46
1:B:277:VAL:CG2	1:B:278:ARG:N	2.80	0.45
1:A:275:PHE:N	1:A:275:PHE:CD1	2.84	0.45
1:B:214:CYS:HB2	1:B:219:ASN:ND2	2.31	0.45
1:B:26:TYR:HA	1:B:64:VAL:O	2.16	0.45
1:A:30:ILE:HD11	1:A:40:HIS:CD2	2.51	0.45
1:A:356:TYR:O	1:A:360:PHE:HD1	1.99	0.45
1:A:345:ALA:HB1	1:A:354:GLU:HB3	1.99	0.45
1:B:353:PRO:O	1:B:356:TYR:HB2	2.17	0.45
1:B:28:CYS:HB3	3:B:1001:CYS:CB	2.47	0.45
1:A:207:ILE:N	1:A:241:GLN:HE22	2.14	0.45
1:B:26:TYR:HB2	1:B:217:LEU:CD1	2.47	0.45
1:B:137:ALA:O	1:B:140:GLY:N	2.43	0.44
1:B:366:VAL:HG22	1:B:380:MET:HG3	1.99	0.44
1:B:44:PHE:CE1	1:B:65:ARG:HD2	2.53	0.44
1:B:214:CYS:HA	1:B:218:GLY:O	2.16	0.44
1:B:65:ARG:NH1	1:B:65:ARG:HG2	2.29	0.44
1:A:332:PRO:HB3	1:A:383:HIS:HA	2.00	0.44
1:A:205:TRP:HE1	3:A:1000:CYS:HA	1.82	0.44
1:A:117:HIS:CG	1:A:212:MET:HG2	2.52	0.44
1:B:196:SER:O	1:B:198:TRP:N	2.51	0.44
1:B:320:TYR:OH	1:B:394:LEU:HA	2.18	0.43
1:A:65:ARG:HB3	1:A:108:PRO:CG	2.47	0.43
1:B:1:MET:HE3	1:B:14:GLU:OE1	2.17	0.43
1:A:237:ASN:O	1:A:241:GLN:HG3	2.18	0.43
1:B:135:TYR:CZ	1:B:143:MET:HB2	2.53	0.43
1:A:397:GLU:O	1:A:398:PRO:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:O	1:A:126:GLU:HG3	2.18	0.43
1:A:326:THR:HG21	1:A:381:ALA:HB1	2.00	0.43
1:B:135:TYR:C	1:B:135:TYR:CD1	2.91	0.43
1:A:241:GLN:O	1:A:245:ALA:CB	2.67	0.43
1:A:326:THR:HG21	1:A:385:ARG:HH22	1.84	0.43
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.84	0.43
1:B:25:MET:HG3	1:B:223:ILE:HG13	2.00	0.43
1:A:135:TYR:HE2	1:A:145:ASP:HB3	1.83	0.43
1:A:6:ASN:HD22	1:A:7:THR:N	2.17	0.42
1:A:6:ASN:ND2	1:A:254:TRP:H	2.17	0.42
1:A:71:ASP:C	1:A:71:ASP:OD2	2.56	0.42
1:B:196:SER:C	1:B:198:TRP:N	2.70	0.42
1:B:196:SER:O	1:B:199:GLY:N	2.53	0.42
1:B:345:ALA:HB1	1:B:354:GLU:HB3	2.02	0.42
1:A:228:SER:HA	1:A:256:HIS:HB3	2.02	0.42
1:B:154:VAL:HG13	1:B:155:LEU:H	1.83	0.41
1:A:153:GLY:HA2	1:A:236:GLU:CD	2.41	0.41
1:A:56:PHE:HE2	1:A:343:ILE:HD11	1.85	0.41
1:A:6:ASN:ND2	1:A:8:LEU:H	2.17	0.41
1:B:252:ASN:HB3	1:B:253:TYR:CD1	2.56	0.41
1:B:262:VAL:O	1:B:263:ASP:CB	2.69	0.41
1:A:115:THR:HG23	1:A:194:TRP:CZ2	2.56	0.41
1:B:115:THR:CG2	1:B:115:THR:O	2.68	0.41
1:A:64:VAL:HG22	1:A:110:MET:HB2	2.03	0.41
1:B:224:HIS:CG	1:B:254:TRP:CZ3	3.08	0.41
1:A:149:ASP:HA	1:A:150:PRO:HD2	1.96	0.41
1:A:330:VAL:HG21	1:A:378:ASN:HB3	2.02	0.41
1:A:3:LYS:HD3	4:A:1023:HOH:O	2.20	0.41
1:B:373:ASP:O	1:B:376:ALA:N	2.54	0.41
1:A:68:THR:HG23	1:A:208:GLU:OE1	2.21	0.40
1:A:32:VAL:HG21	1:A:93:ILE:CG1	2.51	0.40
1:B:143:MET:HE2	1:B:182:VAL:HG22	2.00	0.40
1:A:135:TYR:HE2	1:A:145:ASP:CB	2.34	0.40
1:A:95:GLU:CG	1:A:278:ARG:HH22	2.33	0.40
1:B:110:MET:HA	1:B:110:MET:CE	2.51	0.40
1:B:195:PRO:O	1:B:199:GLY:O	2.39	0.40
1:A:289:VAL:O	1:A:293:LEU:HG	2.21	0.40
1:B:314:ALA:O	1:B:317:GLU:HB2	2.22	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	382/461 (83%)	361 (94%)	14 (4%)	7 (2%)	11	21
1	B	367/461 (80%)	321 (88%)	33 (9%)	13 (4%)	4	6
All	All	749/922 (81%)	682 (91%)	47 (6%)	20 (3%)	6	10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	233	PRO
1	A	263	ASP
1	B	195	PRO
1	B	233	PRO
1	B	264	ARG
1	B	276	THR
1	A	205	TRP
1	A	264	ARG
1	B	266	LYS
1	A	234	HIS
1	B	197	PRO
1	B	234	HIS
1	B	281	LEU
1	B	196	SER
1	B	205	TRP
1	B	274	PHE
1	B	84	SER
1	B	32	VAL
1	A	204	GLY

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	293/381 (77%)	269 (92%)	24 (8%)	14	27
1	B	256/381 (67%)	239 (93%)	17 (7%)	21	40
All	All	549/762 (72%)	508 (92%)	41 (8%)	17	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ASN
1	A	30	ILE
1	A	33	TYR
1	A	34	ASP
1	A	42	ARG
1	A	70	ILE
1	A	75	ILE
1	A	120	GLU
1	A	145	ASP
1	A	146	VAL
1	A	187	SER
1	A	202	ARG
1	A	203	PRO
1	A	214	CYS
1	A	233	PRO
1	A	249	GLN
1	A	271	LEU
1	A	299	ARG
1	A	324	ARG
1	A	329	THR
1	A	357	SER
1	A	380	MET
1	A	398	PRO
1	B	1	MET
1	B	6	ASN
1	B	38	ILE
1	B	42	ARG
1	B	71	ASP
1	B	116	HIS
1	B	195	PRO

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Mol	Chain	Res	Type
1	B	203	PRO
1	B	212	MET
1	B	214	CYS
1	B	216	GLN
1	B	223	ILE
1	B	274	PHE
1	B	278	ARG
1	B	295	SER
1	B	344	GLU
1	B	396	GLN

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	6	ASN
1	A	11	GLN
1	A	37	HIS
1	A	97	HIS
1	A	177	ASN
1	A	219	ASN
1	A	220	HIS
1	A	224	HIS
1	A	235	HIS
1	A	241	GLN
1	A	256	HIS
1	A	297	HIS
1	A	308	ASN
1	A	383	HIS
1	B	6	ASN
1	B	97	HIS
1	B	177	ASN
1	B	219	ASN
1	B	224	HIS
1	B	235	HIS
1	B	241	GLN
1	B	297	HIS
1	B	308	ASN
1	B	383	HIS
1	B	396	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	CYS	A	1000	2	3,6,6	1.92	1 (33%)	1,7,7	2.06	1 (100%)
3	CYS	B	1001	2	3,6,6	1.90	1 (33%)	1,7,7	2.05	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYS	A	1000	2	-	0/2/6/6	0/0/0/0
3	CYS	B	1001	2	-	0/2/6/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	CYS	CB-SG	-3.07	1.74	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	CYS	CB-SG	-3.05	1.74	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	CYS	CA-CB-SG	-2.06	109.77	114.48
3	B	1001	CYS	CA-CB-SG	-2.05	109.79	114.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	CYS	3	0
3	B	1001	CYS	5	0

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	386/461 (83%)	0.14	10 (2%)	59	53	19, 36, 52, 60	0
1	B	375/461 (81%)	0.28	19 (5%)	32	25	22, 45, 68, 93	0
All	All	761/922 (82%)	0.21	29 (3%)	44	36	19, 39, 64, 93	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	3.6
1	B	274	PHE	3.6
1	B	284	TYR	3.3
1	A	135	TYR	3.3
1	B	190	GLY	3.3
1	A	147	PRO	3.2
1	A	146	VAL	3.0
1	A	205	TRP	2.9
1	B	267	MET	2.7
1	A	144	PHE	2.7
1	A	309	LEU	2.7
1	B	263	ASP	2.6
1	B	370	LYS	2.6
1	B	145	ASP	2.4
1	B	264	ARG	2.4
1	B	283	TYR	2.4
1	B	203	PRO	2.3
1	B	136	VAL	2.3
1	A	177	ASN	2.3
1	B	371	ALA	2.2
1	B	325	GLY	2.2
1	B	324	ARG	2.2
1	B	204	GLY	2.2
1	A	153	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	189	GLU	2.2
1	B	262	VAL	2.1
1	B	199	GLY	2.1
1	B	323	LEU	2.0
1	A	180	ASP	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)

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(Å^2)	Q<0.9
3	CYS	B	1001	7/7	0.90	0.22	1.73	49,54,55,56	0
3	CYS	A	1000	7/7	0.93	0.22	0.47	41,47,49,51	0
2	ZN	A	963	1/1	0.92	0.10	-1.40	41,41,41,41	0
2	ZN	B	964	1/1	0.86	0.11	-2.16	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.