Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:51 PM GMT

PDB ID	:	1CTS
Title	:	CRYSTALLOGRAPHIC REFINEMENT AND ATOMIC MODELS OF TWO DIFFERENT FORMS OF CITRATE SYNTHASE AT 2.7 AND 1.7 ANGSTROMS RESOLUTION
Authors	:	Remington, S.; Wiegand, G.; Huber, R.
Deposited on	:	1984-01-27
Resolution	:	2.70 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 (i) symbol.

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

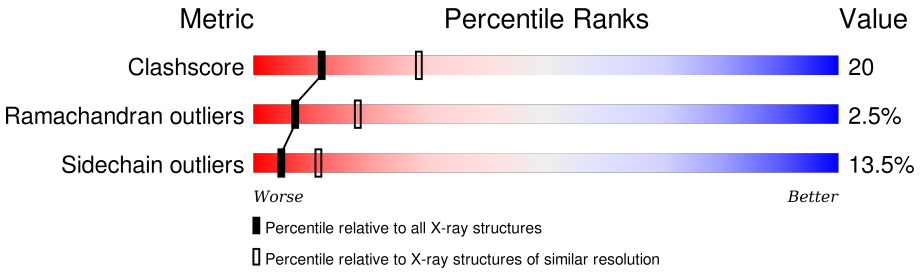
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	47% 37% 13% •

2 Entry composition

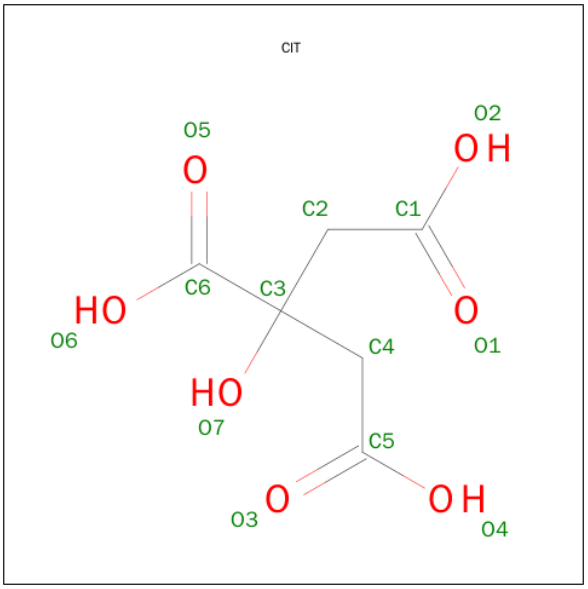
There are 2 unique types of molecules in this entry. The entry contains 3457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	437	3444	2200	591	634	19	132	0	0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0

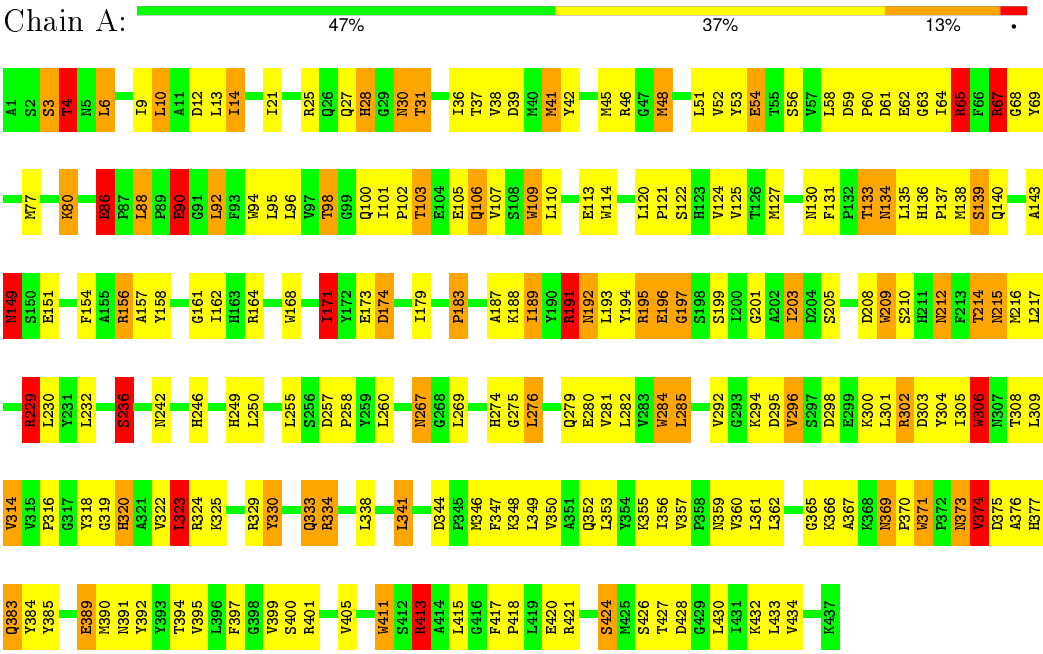
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: CITRATE SYNTHASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.40Å 77.40Å 196.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3457	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.12	11/3528 (0.3%)	1.51	28/4786 (0.6%)

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	A	1	73

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	TRP	NE1-CE2	-8.31	1.26	1.37
1	A	209	TRP	NE1-CE2	-7.88	1.27	1.37
1	A	306	TRP	NE1-CE2	-7.71	1.27	1.37
1	A	94	TRP	NE1-CE2	-7.71	1.27	1.37
1	A	114	TRP	NE1-CE2	-7.64	1.27	1.37
1	A	168	TRP	NE1-CE2	-7.56	1.27	1.37
1	A	284	TRP	NE1-CE2	-7.52	1.27	1.37
1	A	109	TRP	NE1-CE2	-7.46	1.27	1.37
1	A	371	TRP	NE1-CE2	-6.98	1.28	1.37
1	A	304	TYR	CZ-OH	6.39	1.48	1.37
1	A	330	TYR	CZ-OH	5.22	1.46	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	A	195	ARG	NE-CZ-NH2	-8.60	116.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	A	103	THR	N-CA-CB	-7.88	95.32	110.30
1	A	156	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	A	191	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	65	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	301	LEU	N-CA-CB	7.07	124.53	110.40
1	A	229	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	A	196	GLU	N-CA-CB	6.25	121.86	110.60
1	A	156	ARG	N-CA-CB	-6.21	99.43	110.60
1	A	215	ASN	N-CA-CB	-6.18	99.47	110.60
1	A	103	THR	CA-CB-CG2	6.13	120.99	112.40
1	A	413	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	65	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	25	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	330	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	183	PRO	N-CA-CB	5.49	109.88	103.30
1	A	191	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	4	THR	N-CA-CB	5.33	120.43	110.30
1	A	298	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	3	SER	C-N-CA	5.15	134.58	121.70
1	A	276	LEU	N-CA-CB	-5.13	100.14	110.40
1	A	158	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	14	ILE	N-CA-CB	5.07	122.46	110.80
1	A	236	SER	CB-CA-C	-5.04	100.51	110.10
1	A	324	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	334	ARG	NE-CZ-NH1	-5.01	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	71	ILE	CA

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	PRO	Mainchain
1	A	106	GLN	Sidechain
1	A	130	ASN	Sidechain
1	A	133	THR	Mainchain
1	A	134	ASN	Sidechain
1	A	139	SER	Mainchain
1	A	140	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	145	ILE	Mainchain
1	A	149	ASN	Sidechain
1	A	151	GLU	Sidechain
1	A	161	GLY	Mainchain
1	A	171	ILE	Mainchain
1	A	173	GLU	Sidechain
1	A	174	ASP	Sidechain
1	A	179	ILE	Mainchain
1	A	189	ILE	Mainchain
1	A	192	ASN	Sidechain
1	A	196	GLU	Sidechain
1	A	197	GLY	Mainchain
1	A	201	GLY	Mainchain
1	A	203	ILE	Mainchain
1	A	208	ASP	Sidechain,Mainchain,Peptide
1	A	214	THR	Mainchain
1	A	215	ASN	Sidechain
1	A	221	ASP	Sidechain
1	A	226	GLU	Sidechain
1	A	242	ASN	Sidechain
1	A	257	ASP	Sidechain
1	A	267	ASN	Sidechain
1	A	27	GLN	Sidechain
1	A	275	GLY	Mainchain
1	A	276	LEU	Mainchain
1	A	279	GLN	Sidechain
1	A	28	HIS	Mainchain
1	A	280	GLU	Sidechain
1	A	295	ASP	Mainchain
1	A	302	ARG	Mainchain
1	A	31	THR	Mainchain
1	A	310	ASN	Sidechain
1	A	311	SER	Mainchain
1	A	318	TYR	Sidechain
1	A	320	HIS	Mainchain
1	A	323	LEU	Mainchain
1	A	333	GLN	Sidechain
1	A	334	ARG	Sidechain
1	A	352	GLN	Sidechain
1	A	359	ASN	Sidechain
1	A	366	LYS	Mainchain,Peptide
1	A	369	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	373	ASN	Sidechain
1	A	374	VAL	Mainchain
1	A	383	GLN	Sidechain
1	A	385	TYR	Mainchain
1	A	39	ASP	Sidechain
1	A	4	THR	Mainchain,Peptide
1	A	413	ARG	Sidechain
1	A	424	SER	Mainchain
1	A	428	ASP	Mainchain
1	A	48	MET	Mainchain
1	A	53	TYR	Mainchain
1	A	54	GLU	Sidechain
1	A	61	ASP	Mainchain
1	A	62	GLU	Sidechain
1	A	67	ARG	Mainchain
1	A	73	GLU	Sidechain
1	A	80	LYS	Mainchain
1	A	86	GLU	Sidechain
1	A	90	GLU	Sidechain
1	A	98	THR	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	3444	0	3436	133	5
2	A	13	0	5	2	0
All	All	3457	0	3441	134	5

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 20.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HD11	1:A:353:LEU:HD12	1.54	0.90
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.54	0.87
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.56	0.85
1:A:21:ILE:HD12	1:A:415:LEU:HD22	1.55	0.85
1:A:362:LEU:HD13	1:A:370:PRO:HG3	1.58	0.85
1:A:63:GLY:HA2	1:A:323:LEU:HD11	1.61	0.83
1:A:41:MET:HE1	1:A:430:LEU:HD21	1.61	0.81
1:A:146:THR:O	1:A:149:ASN:HB3	1.85	0.76
1:A:98:THR:CG2	1:A:100:GLN:HB2	2.18	0.73
1:A:125:VAL:CG1	1:A:188:LYS:HE2	2.19	0.73
1:A:305:ILE:HD11	1:A:353:LEU:CD1	2.18	0.73
1:A:98:THR:HG22	1:A:100:GLN:HB2	1.69	0.72
1:A:171:ILE:HD12	1:A:413:ARG:HG2	1.70	0.72
1:A:192:ASN:HA	1:A:197:GLY:HA2	1.73	0.70
1:A:362:LEU:HD12	1:A:367:ALA:HB1	1.73	0.70
2:A:438:CIT:O3	2:A:438:CIT:H21	1.91	0.69
1:A:174:ASP:HB3	1:A:258:PRO:HG2	1.74	0.69
1:A:194:TYR:HE2	1:A:392:TYR:HB2	1.59	0.68
1:A:355:LYS:HB3	1:A:356:ILE:HD12	1.75	0.67
1:A:41:MET:HE1	1:A:430:LEU:CD2	2.24	0.67
1:A:63:GLY:H	1:A:323:LEU:HD21	1.61	0.65
1:A:281:VAL:HG11	1:A:376:ALA:HA	1.79	0.65
1:A:189:ILE:O	1:A:193:LEU:HB2	1.96	0.64
1:A:302:ARG:O	1:A:306:TRP:HB2	1.99	0.63
1:A:174:ASP:CB	1:A:258:PRO:HG2	2.28	0.62
1:A:362:LEU:HD12	1:A:367:ALA:CB	2.31	0.61
1:A:133:THR:HG23	1:A:193:LEU:HD12	1.82	0.61
1:A:56:SER:HB2	1:A:64:ILE:HD11	1.83	0.61
1:A:171:ILE:CD1	1:A:413:ARG:HG2	2.30	0.61
1:A:65:ARG:HG2	1:A:68:GLY:HA2	1.83	0.60
1:A:109:TRP:CH2	1:A:113:GLU:HG2	2.36	0.60
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.37	0.59
1:A:320:HIS:O	1:A:369:ASN:HB3	2.02	0.59
1:A:281:VAL:O	1:A:285:LEU:HB2	2.02	0.59
1:A:136:HIS:HD2	1:A:138:MET:H	1.50	0.59
1:A:333:GLN:HB3	1:A:381:LEU:CD2	2.33	0.59
1:A:319:GLY:HA2	1:A:369:ASN:O	2.03	0.59
1:A:64:ILE:HG23	1:A:71:ILE:HD12	1.85	0.59
1:A:349:LEU:O	1:A:353:LEU:HD22	2.04	0.58
1:A:232:LEU:HD23	1:A:400:SER:HB2	1.86	0.58
1:A:77:MET:HB3	1:A:101:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:O	1:A:430:LEU:HG	2.05	0.57
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.86	0.56
1:A:67:ARG:HD3	1:A:69:TYR:CE1	2.39	0.56
1:A:323:LEU:O	1:A:369:ASN:HB2	2.06	0.56
1:A:305:ILE:HG22	1:A:360:VAL:HG11	1.87	0.56
1:A:6:LEU:HA	1:A:9:ILE:HD12	1.88	0.56
1:A:194:TYR:CE2	1:A:392:TYR:HB2	2.41	0.55
1:A:135:LEU:HD11	1:A:139:SER:HB2	1.89	0.55
1:A:274:HIS:CE1	2:A:438:CIT:H41	2.41	0.55
1:A:296:VAL:HG12	1:A:300:LYS:HB3	1.89	0.54
1:A:10:LEU:O	1:A:14:ILE:HG13	2.08	0.54
1:A:309:LEU:CD1	1:A:361:LEU:HD23	2.37	0.54
1:A:135:LEU:HD11	1:A:139:SER:CB	2.38	0.53
1:A:395:VAL:O	1:A:399:VAL:HG23	2.08	0.53
1:A:333:GLN:HB3	1:A:381:LEU:HD21	1.91	0.52
1:A:67:ARG:HD3	1:A:69:TYR:CD1	2.44	0.52
1:A:236:SER:O	1:A:401:ARG:HD3	2.09	0.52
1:A:59:ASP:HB2	1:A:65:ARG:HD3	1.92	0.52
1:A:269:LEU:HD11	1:A:397:PHE:CD2	2.45	0.52
1:A:236:SER:O	1:A:401:ARG:HA	2.10	0.52
1:A:344:ASP:O	1:A:348:LYS:HG3	2.10	0.52
1:A:135:LEU:CD1	1:A:139:SER:HB2	2.40	0.52
1:A:103:THR:HG22	1:A:106:GLN:H	1.74	0.51
1:A:63:GLY:N	1:A:323:LEU:HD21	2.26	0.51
1:A:329:ARG:HB3	1:A:374:VAL:HG13	1.93	0.50
1:A:154:PHE:HZ	1:A:255:LEU:HD22	1.77	0.50
1:A:362:LEU:CD1	1:A:367:ALA:HB1	2.42	0.49
1:A:88:LEU:CD1	1:A:229:ARG:HD2	2.42	0.49
1:A:370:PRO:HD2	1:A:371:TRP:NE1	2.27	0.49
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.42	0.49
1:A:212:ASN:O	1:A:216:MET:HG3	2.13	0.48
1:A:232:LEU:CD2	1:A:400:SER:HB2	2.44	0.48
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.36	0.48
1:A:281:VAL:HG12	1:A:285:LEU:HD22	1.95	0.47
1:A:413:ARG:HA	1:A:413:ARG:NE	2.30	0.47
1:A:329:ARG:CB	1:A:374:VAL:HG13	2.44	0.47
1:A:98:THR:HG21	1:A:100:GLN:HB2	1.92	0.47
1:A:183:PRO:HG3	1:A:209:TRP:NE1	2.30	0.47
1:A:415:LEU:HB2	1:A:417:PHE:CE1	2.50	0.47
1:A:45:MET:HA	1:A:48:MET:HE3	1.97	0.47
1:A:214:THR:HA	1:A:217:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD13	1:A:361:LEU:HD23	1.96	0.46
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.50	0.46
1:A:69:TYR:CE2	1:A:101:ILE:HD11	2.50	0.46
1:A:67:ARG:HB3	1:A:69:TYR:HD1	1.79	0.46
1:A:300:LYS:O	1:A:303:ASP:HB2	2.15	0.45
1:A:194:TYR:CG	1:A:389:GLU:HG2	2.51	0.45
1:A:121:PRO:HG2	1:A:124:VAL:CG2	2.47	0.45
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.78	0.45
1:A:30:ASN:HD22	1:A:30:ASN:HA	1.43	0.45
1:A:187:ALA:O	1:A:191:ARG:HB2	2.17	0.45
1:A:338:LEU:HD23	1:A:347:PHE:CZ	2.52	0.45
1:A:157:ALA:O	1:A:162:ILE:HG12	2.17	0.44
1:A:90:GLU:HB3	1:A:107:VAL:HG13	1.98	0.44
1:A:95:LEU:O	1:A:95:LEU:HG	2.17	0.44
1:A:121:PRO:HG2	1:A:124:VAL:HG23	1.98	0.44
1:A:305:ILE:O	1:A:309:LEU:HG	2.18	0.44
1:A:284:TRP:CG	1:A:316:PRO:HG2	2.53	0.43
1:A:58:LEU:HD23	1:A:322:VAL:HG11	2.01	0.43
1:A:246:HIS:O	1:A:249:HIS:HB3	2.19	0.43
1:A:28:HIS:H	1:A:28:HIS:CD2	2.36	0.43
1:A:38:VAL:O	1:A:42:TYR:HD2	2.01	0.43
1:A:65:ARG:HH11	1:A:70:SER:HB3	1.84	0.43
1:A:333:GLN:NE2	1:A:377:HIS:HB3	2.33	0.43
1:A:92:LEU:O	1:A:92:LEU:HG	2.19	0.42
1:A:60:PRO:O	1:A:323:LEU:HD23	2.20	0.42
1:A:149:ASN:HB2	1:A:260:LEU:HD13	2.01	0.42
1:A:330:TYR:OH	1:A:350:VAL:HG12	2.18	0.42
1:A:10:LEU:HD21	1:A:411:TRP:CZ2	2.55	0.42
1:A:120:LEU:HD23	1:A:125:VAL:HG22	2.01	0.42
1:A:373:ASN:HB3	1:A:375:ASP:H	1.84	0.42
1:A:282:LEU:HD23	1:A:390:MET:HE2	2.00	0.42
1:A:355:LYS:CB	1:A:356:ILE:HD12	2.47	0.42
1:A:36:ILE:HD13	1:A:36:ILE:HG21	1.74	0.42
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.75	0.42
1:A:313:ARG:HB3	1:A:314:VAL:H	1.72	0.41
1:A:433:LEU:HA	1:A:433:LEU:HD12	1.83	0.41
1:A:103:THR:HG22	1:A:105:GLU:H	1.85	0.41
1:A:417:PHE:HA	1:A:418:PRO:HD3	1.93	0.41
1:A:127:MET:HE1	1:A:143:ALA:HB1	2.02	0.41
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.93	0.41
1:A:6:LEU:N	1:A:9:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASP:HB3	1:A:347:PHE:HB3	2.01	0.41
1:A:191:ARG:HA	1:A:195:ARG:HB2	2.02	0.41
1:A:281:VAL:HG22	1:A:316:PRO:HB2	2.02	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.58	0.41
1:A:250:LEU:HD12	1:A:420:GLU:HB3	2.02	0.41
1:A:138:MET:CE	1:A:269:LEU:HD23	2.50	0.40
1:A:174:ASP:HB2	1:A:258:PRO:HG2	2.01	0.40
1:A:110:LEU:HA	1:A:113:GLU:HB3	2.03	0.40
1:A:21:ILE:HD12	1:A:415:LEU:CD2	2.40	0.40
1:A:229:ARG:HD3	1:A:229:ARG:HH11	1.69	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:CG2	1:A:434:VAL:CG2[8_665]	1.46	0.74
1:A:127:MET:CE	1:A:127:MET:CE[8_665]	1.73	0.47
1:A:54:GLU:OE2	1:A:427:THR:OG1[8_665]	1.83	0.37
1:A:139:SER:OG	1:A:149:ASN:ND2[8_665]	1.84	0.36
1:A:31:THR:CB	1:A:434:VAL:CG2[8_665]	1.86	0.34

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	435/437 (100%)	382 (88%)	42 (10%)	11 (2%)	7 18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	67	ARG
1	A	71	ILE
1	A	164	ARG
1	A	294	LYS
1	A	3	SER
1	A	365	GLY
1	A	122	SER
1	A	389	GLU
1	A	52	VAL

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	371/371 (100%)	321 (86%)	50 (14%)	5 11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	10	LEU
1	A	12	ASP
1	A	13	LEU
1	A	30	ASN
1	A	37	THR
1	A	41	MET
1	A	51	LEU
1	A	65	ARG
1	A	80	LYS
1	A	86	GLU
1	A	88	LEU
1	A	90	GLU
1	A	92	LEU
1	A	131	PHE
1	A	134	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	156	ARG
1	A	171	ILE
1	A	191	ARG
1	A	199	SER
1	A	203	ILE
1	A	205	SER
1	A	210	SER
1	A	212	ASN
1	A	229	ARG
1	A	236	SER
1	A	267	ASN
1	A	285	LEU
1	A	292	VAL
1	A	296	VAL
1	A	306	TRP
1	A	308	THR
1	A	310	ASN
1	A	313	ARG
1	A	314	VAL
1	A	323	LEU
1	A	325	LYS
1	A	341	LEU
1	A	346	MET
1	A	374	VAL
1	A	381	LEU
1	A	383	GLN
1	A	391	ASN
1	A	394	THR
1	A	405	VAL
1	A	413	ARG
1	A	421	ARG
1	A	424	SER
1	A	432	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	28	HIS
1	A	30	ASN
1	A	123	HIS

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Mol	Chain	Res	Type
1	A	136	HIS
1	A	140	GLN
1	A	192	ASN
1	A	211	HIS
1	A	215	ASN
1	A	267	ASN
1	A	307	ASN
1	A	352	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)

1 ligand is 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	CIT	A	438	-	3,12,12	1.14	0	3,17,17	3.14	1 (33%)

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	CIT	A	438	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	438	CIT	C3-C4-C5	-5.32	106.44	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	438	CIT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.