Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 07:01 AM JST

PDB ID	:	7F77
Title	:	Crystal structure of glutamate dehydrogenase 3 from Candida albicans
Authors	:	Li, N.; Wang, W.; Zeng, X.; Liu, M.; Li, M.; Li, C.; Wang, M.
Deposited on	:	2021-06-28
Resolution	:	3.09 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 (i) 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 (1)) were used in the production of this report:

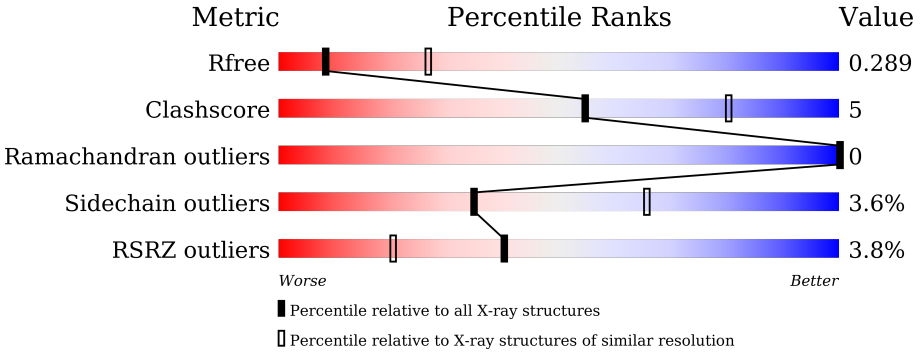
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.09 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}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 <=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	484	.% 75% 13% • 11%
1	B	484	5% 75% 12% 13%
1	C	484	5% 72% 13% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9733 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	3295	2089	556	636	14	0	0	0
1	B	420	3216	2039	543	620	14	0	0	0
1	C	419	3205	2032	539	621	13	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
A	-18	GLY	-	expression tag	UNP A0A1D8PMH8
A	-17	SER	-	expression tag	UNP A0A1D8PMH8
A	-16	SER	-	expression tag	UNP A0A1D8PMH8
A	-15	HIS	-	expression tag	UNP A0A1D8PMH8
A	-14	HIS	-	expression tag	UNP A0A1D8PMH8
A	-13	HIS	-	expression tag	UNP A0A1D8PMH8
A	-12	HIS	-	expression tag	UNP A0A1D8PMH8
A	-11	HIS	-	expression tag	UNP A0A1D8PMH8
A	-10	HIS	-	expression tag	UNP A0A1D8PMH8
A	-9	SER	-	expression tag	UNP A0A1D8PMH8
A	-8	SER	-	expression tag	UNP A0A1D8PMH8
A	-7	GLY	-	expression tag	UNP A0A1D8PMH8
A	-6	LEU	-	expression tag	UNP A0A1D8PMH8
A	-5	VAL	-	expression tag	UNP A0A1D8PMH8
A	-4	PRO	-	expression tag	UNP A0A1D8PMH8
A	-3	ARG	-	expression tag	UNP A0A1D8PMH8
A	-2	GLY	-	expression tag	UNP A0A1D8PMH8
A	-1	SER	-	expression tag	UNP A0A1D8PMH8
A	0	HIS	-	expression tag	UNP A0A1D8PMH8
A	457	LEU	-	expression tag	UNP A0A1D8PMH8
A	458	GLU	-	expression tag	UNP A0A1D8PMH8
A	459	HIS	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP A0A1D8PMH8
A	461	HIS	-	expression tag	UNP A0A1D8PMH8
A	462	HIS	-	expression tag	UNP A0A1D8PMH8
A	463	HIS	-	expression tag	UNP A0A1D8PMH8
A	464	HIS	-	expression tag	UNP A0A1D8PMH8
B	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
B	-18	GLY	-	expression tag	UNP A0A1D8PMH8
B	-17	SER	-	expression tag	UNP A0A1D8PMH8
B	-16	SER	-	expression tag	UNP A0A1D8PMH8
B	-15	HIS	-	expression tag	UNP A0A1D8PMH8
B	-14	HIS	-	expression tag	UNP A0A1D8PMH8
B	-13	HIS	-	expression tag	UNP A0A1D8PMH8
B	-12	HIS	-	expression tag	UNP A0A1D8PMH8
B	-11	HIS	-	expression tag	UNP A0A1D8PMH8
B	-10	HIS	-	expression tag	UNP A0A1D8PMH8
B	-9	SER	-	expression tag	UNP A0A1D8PMH8
B	-8	SER	-	expression tag	UNP A0A1D8PMH8
B	-7	GLY	-	expression tag	UNP A0A1D8PMH8
B	-6	LEU	-	expression tag	UNP A0A1D8PMH8
B	-5	VAL	-	expression tag	UNP A0A1D8PMH8
B	-4	PRO	-	expression tag	UNP A0A1D8PMH8
B	-3	ARG	-	expression tag	UNP A0A1D8PMH8
B	-2	GLY	-	expression tag	UNP A0A1D8PMH8
B	-1	SER	-	expression tag	UNP A0A1D8PMH8
B	0	HIS	-	expression tag	UNP A0A1D8PMH8
B	457	LEU	-	expression tag	UNP A0A1D8PMH8
B	458	GLU	-	expression tag	UNP A0A1D8PMH8
B	459	HIS	-	expression tag	UNP A0A1D8PMH8
B	460	HIS	-	expression tag	UNP A0A1D8PMH8
B	461	HIS	-	expression tag	UNP A0A1D8PMH8
B	462	HIS	-	expression tag	UNP A0A1D8PMH8
B	463	HIS	-	expression tag	UNP A0A1D8PMH8
B	464	HIS	-	expression tag	UNP A0A1D8PMH8
C	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
C	-18	GLY	-	expression tag	UNP A0A1D8PMH8
C	-17	SER	-	expression tag	UNP A0A1D8PMH8
C	-16	SER	-	expression tag	UNP A0A1D8PMH8
C	-15	HIS	-	expression tag	UNP A0A1D8PMH8
C	-14	HIS	-	expression tag	UNP A0A1D8PMH8
C	-13	HIS	-	expression tag	UNP A0A1D8PMH8
C	-12	HIS	-	expression tag	UNP A0A1D8PMH8
C	-11	HIS	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP A0A1D8PMH8
C	-9	SER	-	expression tag	UNP A0A1D8PMH8
C	-8	SER	-	expression tag	UNP A0A1D8PMH8
C	-7	GLY	-	expression tag	UNP A0A1D8PMH8
C	-6	LEU	-	expression tag	UNP A0A1D8PMH8
C	-5	VAL	-	expression tag	UNP A0A1D8PMH8
C	-4	PRO	-	expression tag	UNP A0A1D8PMH8
C	-3	ARG	-	expression tag	UNP A0A1D8PMH8
C	-2	GLY	-	expression tag	UNP A0A1D8PMH8
C	-1	SER	-	expression tag	UNP A0A1D8PMH8
C	0	HIS	-	expression tag	UNP A0A1D8PMH8
C	457	LEU	-	expression tag	UNP A0A1D8PMH8
C	458	GLU	-	expression tag	UNP A0A1D8PMH8
C	459	HIS	-	expression tag	UNP A0A1D8PMH8
C	460	HIS	-	expression tag	UNP A0A1D8PMH8
C	461	HIS	-	expression tag	UNP A0A1D8PMH8
C	462	HIS	-	expression tag	UNP A0A1D8PMH8
C	463	HIS	-	expression tag	UNP A0A1D8PMH8
C	464	HIS	-	expression tag	UNP A0A1D8PMH8

- Molecule 2 is water.

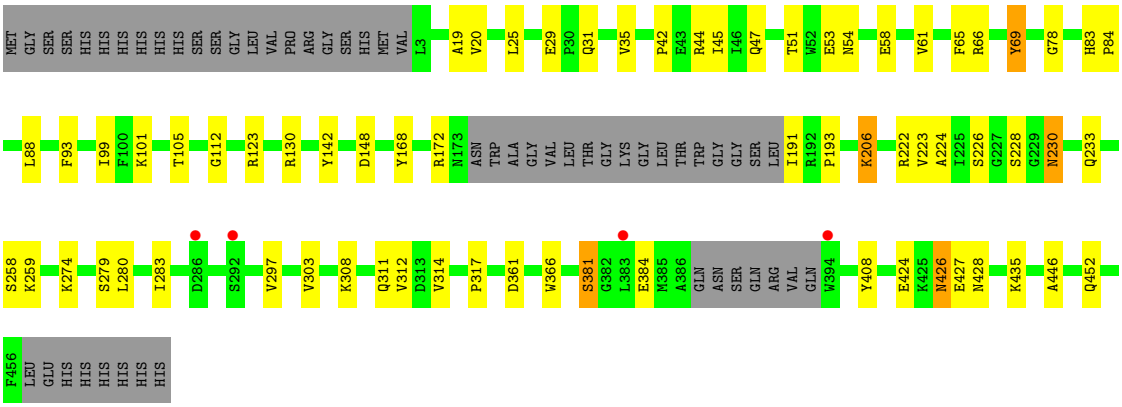
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	11	11	11	0	0
			Total	O		
2	B	3	3	3	0	0
			Total	O		
2	C	3	3	3	0	0

3 Residue-property plots (i)

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.

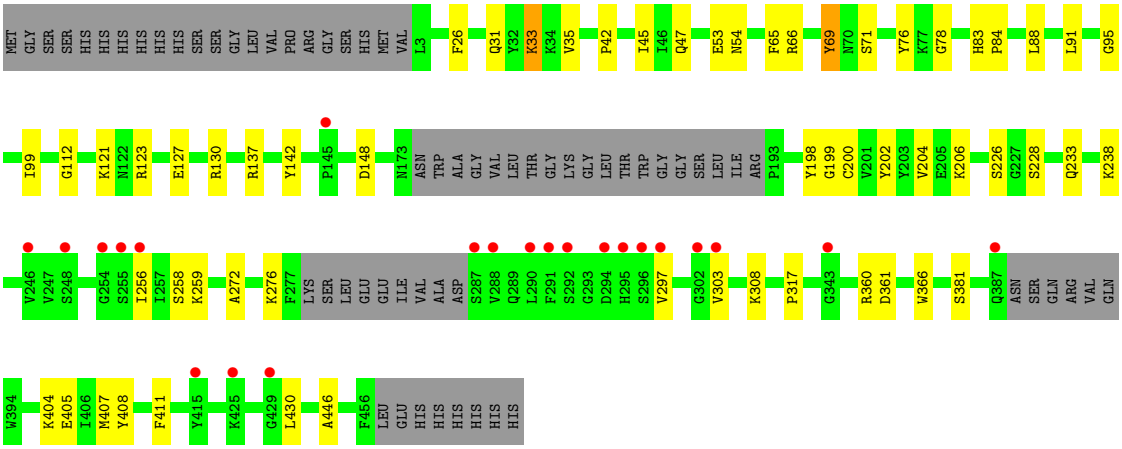
• Molecule 1: Glutamate dehydrogenase

Chain A:



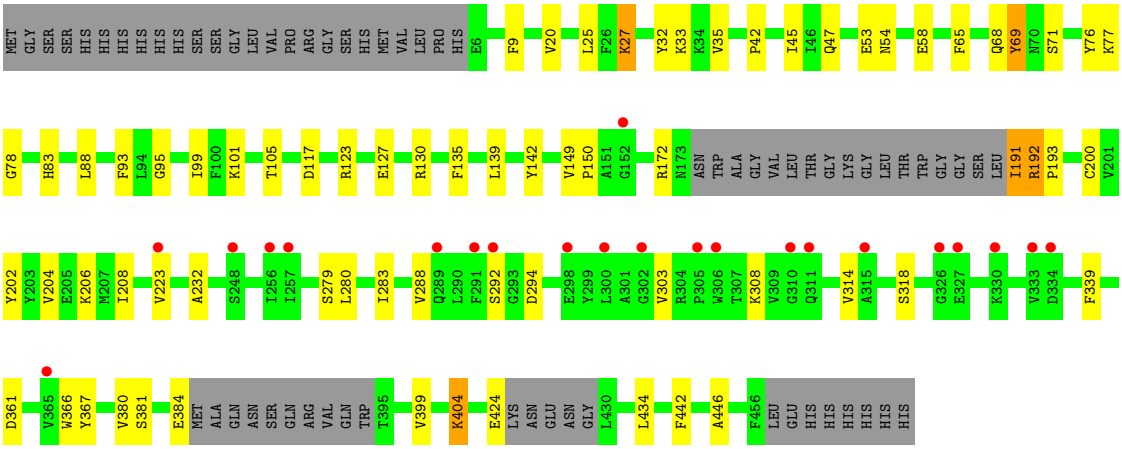
• Molecule 1: Glutamate dehydrogenase

Chain B:



• Molecule 1: Glutamate dehydrogenase

Chain C:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET VAL LEU PRO HIS E6
F9
V20
L25 F26 K27
Y32 K33 K34 V35
P42
I45 I46 Q47
E53 N54
E58
F65
Q68 Y69 N70 S71
Y76 K77
G78
H83
L88
F93 L94 G95
I99 F100 K101
T105
D117
R123
E127
R130
F135
L139
Y142
V149 P150 A151 G152
R172 N173 ASN TRP ALA GLY VAL LEU THR GLY LYS GLY LEU THR TRP GLY GLY SER LEU I191 R192 P193
C200 V201
Y202 Y203 V204 E205 K206 M207 I208
V223
A232
S248
I256 I257
S279 L280
I283
V288
Q289 L290 F291 S292 G293 D294
E298 Y299 L300 A301 G302
V303 R304 P305 W306 T307 K308 V309 G310 Q311
V314 A315
S318
G326 E327
K330
V333 D334
F339
D361
V365 W366 Y367
V380 S381
E384 MET ALA GLN ASN SER GLN ARG VAL GLN TRP T395
V399
K404
E424 LYS ASN GLU ASN GLY L430
L434
F442
A446
F456 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.54Å 94.54Å 334.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.52 – 3.09 43.52 – 3.09	Depositor EDS
% Data completeness (in resolution range)	83.8 (43.52-3.09) 83.8 (43.52-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.241 , 0.290 0.241 , 0.289	Depositor DCC
R_{free} test set	1155 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 26.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.28	0/3356	0.45	0/4524
1	B	0.28	0/3276	0.43	0/4414
1	C	0.27	0/3261	0.44	0/4393
All	All	0.28	0/9893	0.44	0/13331

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 (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	3295	0	3251	36	0
1	B	3216	0	3165	29	0
1	C	3205	0	3167	36	0
2	A	11	0	0	1	0
2	B	3	0	0	1	0
2	C	3	0	0	0	0
All	All	9733	0	9583	101	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 5.

All (101) 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:193:PRO:O	1:A:230:ASN:ND2	2.21	0.74
1:B:45:ILE:HD13	1:B:88:LEU:HD11	1.78	0.65
1:C:78:GLY:O	1:C:150:PRO:HA	1.99	0.63
1:A:45:ILE:HD13	1:A:88:LEU:HD11	1.83	0.61
1:C:45:ILE:HD13	1:C:88:LEU:HD11	1.84	0.59
1:C:42:PRO:HG2	1:C:45:ILE:HD11	1.84	0.59
1:A:51:THR:HG22	1:A:61:VAL:HG22	1.87	0.57
1:B:42:PRO:HG2	1:B:45:ILE:HD11	1.87	0.56
1:B:66:ARG:NH2	1:B:148:ASP:OD1	2.36	0.56
1:C:191:ILE:HD12	1:C:399:VAL:HG21	1.88	0.55
1:A:452:GLN:NE2	2:A:501:HOH:O	2.39	0.55
1:C:279:SER:O	1:C:283:ILE:HG23	2.08	0.54
1:A:381:SER:O	1:A:384:GLU:HB3	2.08	0.54
1:A:303:VAL:HG11	1:A:308:LYS:HE3	1.89	0.54
1:C:71:SER:HB3	1:C:76:TYR:CE1	2.43	0.53
1:B:35:VAL:HG21	1:B:446:ALA:HB1	1.91	0.53
1:B:303:VAL:HG11	1:B:308:LYS:HE3	1.89	0.53
1:B:272:ALA:O	1:B:276:LYS:HG2	2.10	0.52
1:A:69:TYR:CD1	1:A:99:ILE:HD11	2.44	0.52
1:A:168:TYR:CE1	1:A:172:ARG:HG3	2.45	0.52
1:B:53:GLU:O	1:B:130:ARG:HD2	2.09	0.52
1:C:303:VAL:HG11	1:C:308:LYS:HE3	1.92	0.52
1:A:78:GLY:HA3	1:A:112:GLY:O	2.10	0.52
1:C:223:VAL:HG22	1:C:314:VAL:HB	1.92	0.52
1:A:206:LYS:HG2	1:A:408:TYR:CD1	2.45	0.51
1:B:228:SER:O	1:B:233:GLN:NE2	2.40	0.51
1:A:426:ASN:N	1:A:426:ASN:OD1	2.43	0.51
1:B:95:GLY:O	1:B:99:ILE:HG13	2.11	0.51
1:C:77:LYS:HD2	1:C:149:VAL:HB	1.94	0.50
1:C:53:GLU:O	1:C:130:ARG:HD2	2.11	0.50
1:B:78:GLY:HA3	1:B:112:GLY:O	2.12	0.49
1:C:27:LYS:HD2	1:C:27:LYS:H	1.77	0.49
1:C:47:GLN:HG2	1:C:65:PHE:CD2	2.48	0.49
1:C:380:VAL:O	1:C:384:GLU:HG2	2.13	0.48
1:C:35:VAL:HG21	1:C:446:ALA:HB1	1.94	0.48
1:A:258:SER:HB3	1:A:297:VAL:HG12	1.96	0.48
1:A:42:PRO:HG2	1:A:45:ILE:HD11	1.95	0.48
1:C:32:TYR:HB3	1:C:442:PHE:HE2	1.79	0.47
1:B:200:CYS:O	1:B:204:VAL:HG23	2.15	0.47
1:B:404:LYS:HG2	1:B:408:TYR:CZ	2.49	0.47
1:A:279:SER:O	1:A:283:ILE:HG23	2.13	0.47
1:B:258:SER:HB3	1:B:297:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:HIS:O	1:C:117:ASP:HA	2.16	0.46
1:C:54:ASN:HA	1:C:127:GLU:HG2	1.96	0.46
1:B:199:GLY:HA2	1:B:407:MET:HG3	1.97	0.46
1:B:54:ASN:HA	1:B:127:GLU:HG2	1.97	0.46
1:C:69:TYR:CD1	1:C:99:ILE:HD11	2.51	0.46
1:A:47:GLN:HG2	1:A:65:PHE:CD2	2.51	0.46
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.51	0.45
1:B:47:GLN:NE2	2:B:501:HOH:O	2.44	0.45
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.56	0.45
1:C:101:LYS:O	1:C:105:THR:HG23	2.16	0.45
1:C:95:GLY:O	1:C:99:ILE:HG13	2.16	0.45
1:A:20:VAL:HG13	1:A:25:LEU:HD23	1.99	0.45
1:A:228:SER:OG	1:A:274:LYS:HE3	2.17	0.45
1:C:20:VAL:HG13	1:C:25:LEU:HD23	1.99	0.45
1:C:202:TYR:CD2	1:C:404:LYS:HG3	2.52	0.44
1:B:69:TYR:CD1	1:B:99:ILE:HD11	2.52	0.44
1:C:232:ALA:HB2	1:C:318:SER:HB2	2.00	0.44
1:A:44:ARG:HB2	1:A:44:ARG:CZ	2.47	0.44
1:A:228:SER:O	1:A:233:GLN:NE2	2.46	0.44
1:C:280:LEU:O	1:C:283:ILE:HG13	2.17	0.44
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.52	0.44
1:B:206:LYS:HB3	1:B:411:PHE:CD2	2.53	0.44
1:C:208:ILE:HG12	1:C:339:PHE:CE2	2.53	0.43
1:A:191:ILE:HG22	1:A:193:PRO:HD2	2.00	0.43
1:A:35:VAL:HG21	1:A:446:ALA:HB1	2.00	0.43
1:A:29:GLU:HG2	1:A:31:GLN:HE22	1.82	0.43
1:C:200:CYS:O	1:C:204:VAL:HG23	2.18	0.43
1:A:280:LEU:O	1:A:283:ILE:HG13	2.18	0.43
1:C:192:ARG:N	1:C:193:PRO:CD	2.82	0.43
1:B:71:SER:HB3	1:B:76:TYR:CE1	2.55	0.42
1:A:19:ALA:HB1	1:A:435:LYS:HA	2.01	0.42
1:A:226:SER:OG	1:A:317:PRO:HA	2.19	0.42
1:B:47:GLN:HG2	1:B:65:PHE:CD2	2.55	0.42
1:A:223:VAL:HG22	1:A:314:VAL:HB	2.01	0.42
1:A:53:GLU:O	1:A:130:ARG:HD2	2.19	0.42
1:A:259:LYS:HE2	1:A:259:LYS:HB3	1.90	0.41
1:C:192:ARG:N	1:C:193:PRO:HD3	2.34	0.41
1:C:206:LYS:HD3	1:C:206:LYS:HA	1.70	0.41
1:A:222:ARG:NE	1:A:311:GLN:O	2.48	0.41
1:B:226:SER:OG	1:B:317:PRO:HA	2.20	0.41
1:C:9:PHE:N	1:C:93:PHE:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:HB	1:B:297:VAL:HG11	2.02	0.41
1:B:202:TYR:CZ	1:B:404:LYS:HE2	2.56	0.41
1:A:66:ARG:NH2	1:A:148:ASP:OD1	2.45	0.41
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.93	0.41
1:B:360:ARG:HD2	1:B:430:LEU:O	2.21	0.41
1:C:367:TYR:HE2	1:C:434:LEU:HD13	1.86	0.41
1:A:424:GLU:HB2	1:A:427:GLU:HB2	2.01	0.41
1:C:42:PRO:HG3	1:C:69:TYR:CZ	2.56	0.41
1:C:68:GLN:HB3	1:C:76:TYR:CE1	2.55	0.41
1:B:26:PHE:CE2	1:B:33:LYS:HE3	2.57	0.40
1:B:202:TYR:CD2	1:B:404:LYS:HG3	2.56	0.40
1:B:198:TYR:CD1	1:B:238:LYS:HB2	2.57	0.40
1:C:135:PHE:CE2	1:C:139:LEU:HD22	2.55	0.40
1:C:288:VAL:O	1:C:292:SER:HB2	2.21	0.40
1:A:54:ASN:HD21	1:A:58:GLU:HB2	1.85	0.40
1:A:101:LYS:O	1:A:105:THR:HG23	2.22	0.40
1:A:224:ALA:HB2	1:A:312:VAL:HG21	2.03	0.40
1:C:54:ASN:HD21	1:C:58:GLU:HB2	1.86	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	424/484 (88%)	412 (97%)	12 (3%)	0	100	100
1	B	412/484 (85%)	402 (98%)	10 (2%)	0	100	100
1	C	411/484 (85%)	401 (98%)	10 (2%)	0	100	100
All	All	1247/1452 (86%)	1215 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	346/391 (88%)	335 (97%)	11 (3%)	39	68
1	B	337/391 (86%)	325 (96%)	12 (4%)	35	66
1	C	337/391 (86%)	323 (96%)	14 (4%)	30	61
All	All	1020/1173 (87%)	983 (96%)	37 (4%)	35	66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	TYR
1	A	93	PHE
1	A	123	ARG
1	A	142	TYR
1	A	206	LYS
1	A	230	ASN
1	A	361	ASP
1	A	366	TRP
1	A	381	SER
1	A	426	ASN
1	A	428	ASN
1	B	31	GLN
1	B	33	LYS
1	B	69	TYR
1	B	121	LYS
1	B	123	ARG
1	B	137	ARG
1	B	142	TYR
1	B	259	LYS
1	B	361	ASP
1	B	366	TRP
1	B	381	SER
1	B	405	GLU
1	C	27	LYS
1	C	33	LYS
1	C	69	TYR

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Mol	Chain	Res	Type
1	C	123	ARG
1	C	142	TYR
1	C	172	ARG
1	C	191	ILE
1	C	192	ARG
1	C	294	ASP
1	C	361	ASP
1	C	366	TRP
1	C	381	SER
1	C	404	LYS
1	C	424	GLU

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

Mol	Chain	Res	Type
1	A	138	GLN
1	B	10	GLN
1	B	138	GLN
1	C	98	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	430/484 (88%)	-0.20	4 (0%)	84	68	21, 38, 78, 93	0
1	B	420/484 (86%)	0.22	22 (5%)	27	12	25, 68, 123, 145	0
1	C	419/484 (86%)	0.11	22 (5%)	26	12	27, 64, 103, 122	0
All	All	1269/1452 (87%)	0.04	48 (3%)	40	20	21, 53, 108, 145	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	PHE	4.8
1	C	311	GLN	4.4
1	B	292	SER	4.0
1	C	306	TRP	3.9
1	C	326	GLY	3.8
1	B	295	HIS	3.8
1	B	297	VAL	3.6
1	B	290	LEU	3.5
1	C	298	GLU	3.5
1	A	394	TRP	3.4
1	C	248	SER	3.4
1	B	429	GLY	3.3
1	C	289	GLN	3.3
1	B	255	SER	3.3
1	B	246	VAL	3.3
1	B	296	SER	3.0
1	C	310	GLY	2.9
1	B	248	SER	2.8
1	B	387	GLN	2.8
1	B	294	ASP	2.8
1	B	303	VAL	2.8
1	C	256	ILE	2.7
1	B	288	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLY	2.7
1	C	315	ALA	2.7
1	B	145	PRO	2.7
1	C	300	LEU	2.6
1	B	287	SER	2.6
1	B	256	ILE	2.5
1	C	333	VAL	2.5
1	C	291	PHE	2.5
1	C	223	VAL	2.5
1	C	365	VAL	2.4
1	C	305	PRO	2.4
1	C	152	GLY	2.3
1	C	302	GLY	2.3
1	C	330	LYS	2.3
1	C	327	GLU	2.1
1	C	292	SER	2.1
1	B	302	GLY	2.1
1	C	257	ILE	2.1
1	A	383	LEU	2.1
1	A	292	SER	2.1
1	B	425	LYS	2.0
1	A	286	ASP	2.0
1	C	334	ASP	2.0
1	B	254	GLY	2.0
1	B	415	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.