Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:26 AM GMT

PDB ID	:	3IH8
Title	:	Crystal Structure Analysis of Mglu in its native form
Authors	:	Yoshimune, K.; Shirakihara, Y.
Deposited on	:	2009-07-29
Resolution	:	2.30 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 (1)) were used in the production of this report:

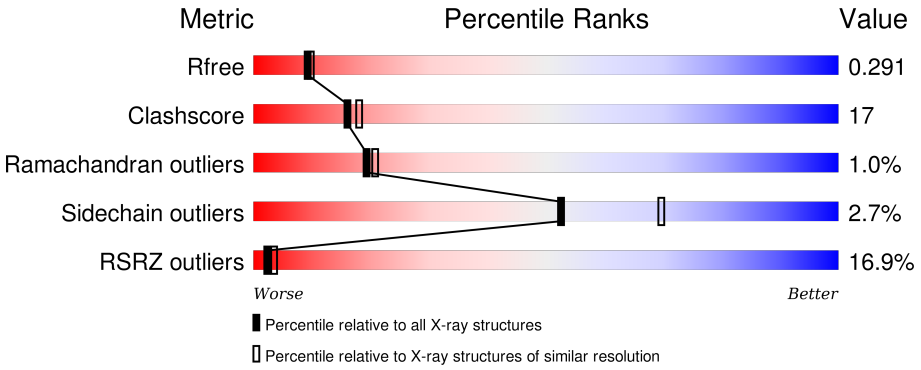
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	456	16% 65% 24% • 9%
1	B	456	15% 64% 24% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6549 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 Salt-tolerant glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3070	1907	561	587	15			
1	B	411	Total	C	N	O	S	0	0	0
			3046	1892	557	582	15			

- Molecule 2 is water.

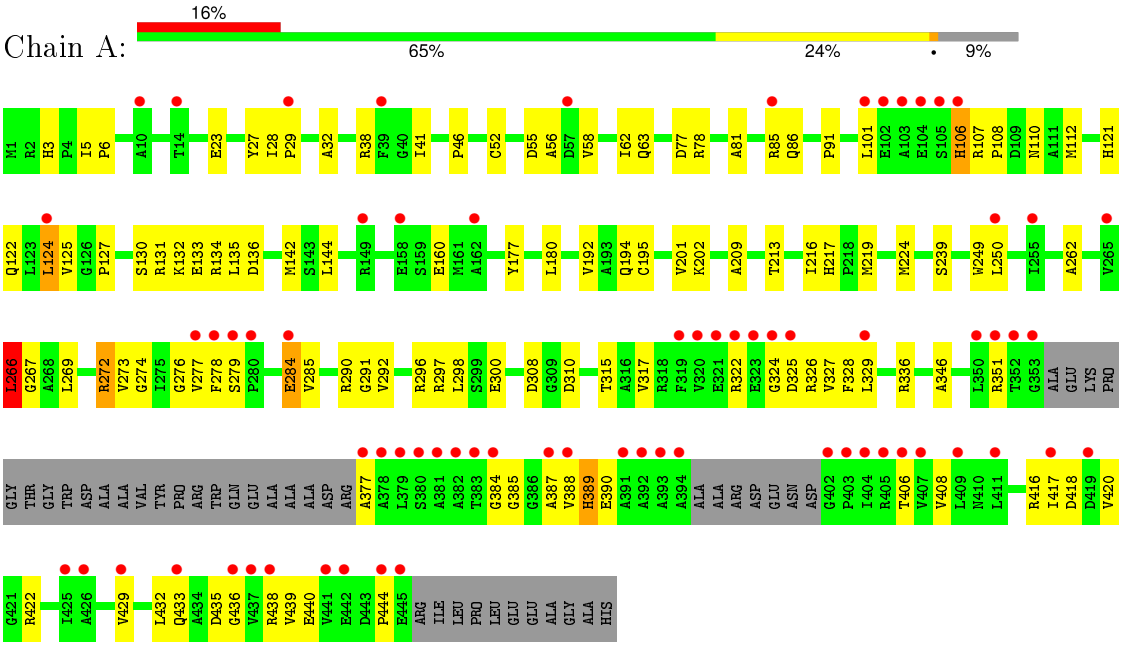
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	226	Total	O	0	0
			226	226		
2	B	207	Total	O	0	0
			207	207		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

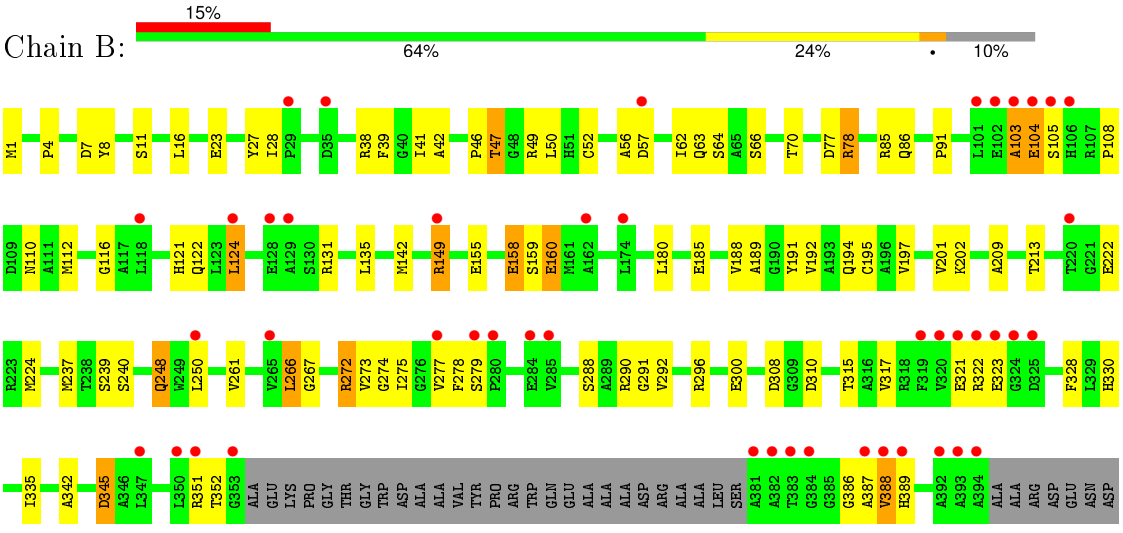
- Molecule 1: Salt-tolerant glutaminase

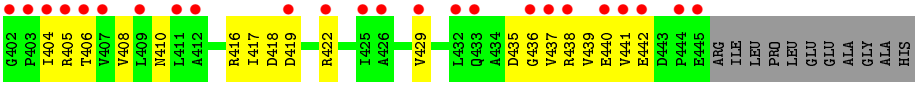
Chain A:



- Molecule 1: Salt-tolerant glutaminase

Chain B:




G402
P403
T404
R405
T406
V407
V408
L409
N410
L411
A412
R416
I417
D418
D419
R422
I425
A426
V429
L432
Q433
A434
D435
G436
V437
R438
V439
E440
V441
E442
D443
P444
E445
ARG
ILE
LEU
PRO
LEU
GLU
GLU
ALA
GLY
ALA
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.08Å 142.25Å 74.25Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	19.90 – 2.30 19.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.90-2.30) 100.0 (19.90-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.30Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.247 , 0.291 0.247 , 0.291	Depositor DCC
R_{free} test set	2620 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 70.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 52579 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6549	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.74 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3606e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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	0.35	0/3114	0.61	2/4222 (0.0%)
1	B	0.34	0/3090	0.62	1/4189 (0.0%)
All	All	0.34	0/6204	0.62	3/8411 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	LEU	N-CA-C	6.09	127.44	111.00
1	B	124	LEU	N-CA-C	5.95	127.05	111.00
1	A	266	LEU	CA-CB-CG	5.39	127.71	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3070	100	0
1	B	3046	0	3044	107	0
2	A	226	0	0	14	0
2	B	207	0	0	17	0
All	All	6549	0	6114	207	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 17.

All (207) 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:110:ASN:HD22	1:B:112:MET:H	1.10	0.95
1:A:62:ILE:HG21	1:A:142:MET:HE1	1.50	0.93
1:A:110:ASN:HD22	1:A:112:MET:H	1.26	0.82
1:A:272:ARG:NH2	1:A:308:ASP:HB2	1.95	0.81
1:B:422:ARG:HD3	2:B:560:HOH:O	1.84	0.76
1:A:269:LEU:HD21	1:A:272:ARG:NH1	2.02	0.75
1:B:279:SER:OG	1:B:290:ARG:HD3	1.87	0.74
1:B:272:ARG:NH2	1:B:308:ASP:OD1	2.21	0.73
1:A:201:VAL:HG23	2:A:457:HOH:O	1.87	0.73
1:A:310:ASP:HB3	2:A:477:HOH:O	1.89	0.73
1:A:406:THR:OG1	1:A:438:ARG:HB3	1.89	0.73
1:A:23:GLU:HA	2:A:517:HOH:O	1.88	0.72
1:A:249:TRP:HZ3	1:A:292:VAL:HG13	1.54	0.72
1:B:78:ARG:HH11	1:B:78:ARG:HB3	1.54	0.71
1:B:110:ASN:ND2	1:B:112:MET:H	1.86	0.70
1:B:405:ARG:HH22	1:B:437:VAL:HA	1.56	0.70
1:A:336:ARG:HA	1:A:418:ASP:OD1	1.92	0.69
1:A:272:ARG:NH2	1:A:308:ASP:CB	2.57	0.68
1:B:63:GLN:HA	1:B:195:CYS:HB3	1.76	0.67
1:B:121:HIS:HD2	1:B:194:GLN:OE1	1.78	0.67
1:B:1:MET:HG2	2:B:520:HOH:O	1.93	0.67
1:A:408:VAL:HG22	1:A:440:GLU:HG3	1.78	0.66
1:B:296:ARG:O	1:B:300:GLU:HG3	1.95	0.65
1:B:38:ARG:HD3	2:B:589:HOH:O	1.95	0.65
1:A:201:VAL:HG13	1:A:276:GLY:C	2.17	0.65
1:A:277:VAL:HG11	1:A:291:GLY:HA2	1.79	0.65
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.60	0.65
1:A:101:LEU:O	1:A:106:HIS:HA	1.96	0.65
1:B:27:TYR:CD1	1:B:28:ILE:HG23	2.31	0.64
1:B:62:ILE:HG21	1:B:142:MET:HE1	1.80	0.64
1:B:310:ASP:HB3	2:B:554:HOH:O	1.97	0.64
1:A:429:VAL:HG13	1:A:439:VAL:HG11	1.78	0.64
1:A:62:ILE:HD13	1:A:142:MET:HE3	1.79	0.64
1:B:160:GLU:HG2	1:B:192:VAL:HG13	1.80	0.64
1:A:296:ARG:O	1:A:300:GLU:HG3	1.98	0.63
1:A:310:ASP:HA	2:A:551:HOH:O	1.97	0.63
1:B:405:ARG:NE	1:B:405:ARG:HA	2.14	0.63
1:A:27:TYR:CD1	1:A:28:ILE:HG23	2.35	0.62
1:A:377:ALA:N	2:A:527:HOH:O	2.32	0.62
1:B:155:GLU:O	1:B:158:GLU:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TRP:CZ3	1:A:292:VAL:HG13	2.36	0.61
1:A:406:THR:HA	1:A:438:ARG:O	2.01	0.60
1:A:420:VAL:HG23	2:A:479:HOH:O	2.02	0.60
1:B:52:CYS:SG	1:B:202:LYS:HE2	2.41	0.60
1:A:216:ILE:HD12	1:A:416:ARG:NH2	2.17	0.60
1:A:326:ARG:HD3	1:A:328:PHE:CZ	2.37	0.60
1:B:62:ILE:CD1	1:B:142:MET:HE3	2.32	0.59
1:A:52:CYS:SG	1:A:202:LYS:HE2	2.43	0.59
1:B:104:GLU:HG2	2:B:514:HOH:O	2.02	0.58
1:B:160:GLU:HG2	1:B:192:VAL:CG1	2.33	0.58
1:B:422:ARG:HG2	1:B:422:ARG:HH11	1.67	0.58
1:B:62:ILE:HD13	1:B:142:MET:HE3	1.85	0.58
1:A:273:VAL:HG22	1:A:274:GLY:N	2.19	0.58
1:B:405:ARG:NH2	1:B:436:GLY:O	2.35	0.58
1:A:417:ILE:HG23	1:A:422:ARG:HG2	1.85	0.58
1:A:160:GLU:HG2	1:A:192:VAL:HG13	1.86	0.57
1:B:322:ARG:NH2	1:B:404:ILE:HG12	2.19	0.57
1:A:144:LEU:HB3	1:A:224:MET:CE	2.35	0.57
1:B:50:LEU:HD21	1:B:202:LYS:HB3	1.87	0.56
1:A:38:ARG:HG2	2:A:667:HOH:O	2.06	0.56
1:B:408:VAL:HG22	1:B:440:GLU:HG3	1.86	0.56
1:B:345:ASP:HB2	2:B:493:HOH:O	2.05	0.55
1:B:419:ASP:HA	1:B:422:ARG:HD2	1.89	0.55
1:A:279:SER:OG	1:A:290:ARG:HD2	2.06	0.55
1:B:104:GLU:N	2:B:481:HOH:O	2.40	0.54
1:A:262:ALA:HB3	2:A:458:HOH:O	2.07	0.54
1:B:273:VAL:HG22	1:B:274:GLY:N	2.21	0.54
1:A:91:PRO:HB3	1:A:239:SER:O	2.07	0.54
1:B:110:ASN:O	1:B:116:GLY:HA3	2.07	0.54
1:B:201:VAL:HG13	2:B:458:HOH:O	2.06	0.54
1:A:62:ILE:CD1	1:A:142:MET:HE3	2.38	0.54
1:B:85:ARG:HD2	1:B:86:GLN:OE1	2.07	0.54
1:A:41:ILE:HA	1:A:201:VAL:HG11	1.90	0.53
1:B:201:VAL:HG12	1:B:278:PHE:HB2	1.90	0.53
1:A:422:ARG:HB3	1:A:422:ARG:NH1	2.24	0.53
1:B:405:ARG:CZ	1:B:405:ARG:HA	2.38	0.53
1:A:41:ILE:HD11	1:A:298:LEU:HD11	1.89	0.53
1:B:185:GLU:CD	1:B:185:GLU:H	2.12	0.53
1:B:222:GLU:O	1:B:224:MET:HE3	2.09	0.53
1:A:272:ARG:HH22	1:A:308:ASP:CB	2.22	0.53
1:B:110:ASN:HD22	1:B:112:MET:N	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.21	0.52
1:A:322:ARG:HG2	1:A:322:ARG:HH21	1.75	0.52
1:B:77:ASP:OD2	1:B:124:LEU:O	2.28	0.52
1:B:47:THR:OG1	1:B:49:ARG:NH1	2.43	0.52
1:B:422:ARG:HG2	1:B:422:ARG:NH1	2.23	0.52
1:B:416:ARG:NH1	2:B:659:HOH:O	2.42	0.52
1:B:158:GLU:HG3	1:B:159:SER:H	1.75	0.51
1:A:417:ILE:CG2	1:A:422:ARG:HG2	2.40	0.51
1:B:272:ARG:NH2	1:B:308:ASP:HB2	2.25	0.51
1:B:330:HIS:CD2	1:B:410:ASN:HB3	2.45	0.51
1:B:209:ALA:O	1:B:213:THR:HG23	2.10	0.51
1:A:124:LEU:HB2	1:A:134:ARG:HG2	1.92	0.51
1:A:135:LEU:HD23	1:A:135:LEU:O	2.10	0.51
1:A:125:VAL:N	2:A:563:HOH:O	2.05	0.51
1:A:110:ASN:ND2	1:A:112:MET:HB2	2.26	0.51
1:A:77:ASP:OD2	1:A:124:LEU:O	2.30	0.50
1:A:217:HIS:HE1	1:A:219:MET:HG2	1.74	0.50
1:A:130:SER:OG	1:A:133:GLU:HG3	2.11	0.50
1:A:121:HIS:HD2	1:A:194:GLN:OE1	1.94	0.50
1:A:317:VAL:O	1:A:387:ALA:HB3	2.12	0.50
1:B:110:ASN:ND2	1:B:112:MET:HB2	2.27	0.50
1:B:41:ILE:HG12	1:B:277:VAL:HG13	1.94	0.50
1:B:248:GLN:NE2	2:B:490:HOH:O	2.45	0.49
1:A:62:ILE:HD13	1:A:142:MET:CE	2.42	0.49
1:B:405:ARG:NH2	1:B:437:VAL:HA	2.27	0.49
1:B:23:GLU:HA	2:B:468:HOH:O	2.12	0.49
1:A:132:LYS:HD3	1:A:136:ASP:OD2	2.13	0.49
1:B:322:ARG:HH22	1:B:404:ILE:HG12	1.78	0.49
1:A:63:GLN:HA	1:A:195:CYS:HB3	1.93	0.49
1:B:441:VAL:HB	2:B:624:HOH:O	2.13	0.49
1:B:158:GLU:HG3	1:B:159:SER:N	2.28	0.48
1:A:440:GLU:OE1	2:A:646:HOH:O	2.20	0.48
1:A:279:SER:OG	1:A:290:ARG:CD	2.62	0.48
1:A:322:ARG:HD3	1:A:327:VAL:HG22	1.95	0.48
1:B:267:GLY:HA3	1:B:275:ILE:HB	1.96	0.48
1:A:417:ILE:HG23	1:A:422:ARG:CG	2.43	0.48
1:B:352:THR:OG1	1:B:435:ASP:OD2	2.31	0.47
1:A:86:GLN:O	1:A:108:PRO:HD2	2.13	0.47
1:A:122:GLN:HB2	1:A:180:LEU:HD22	1.96	0.47
1:A:29:PRO:HA	1:A:32:ALA:HB3	1.95	0.47
1:A:144:LEU:HB3	1:A:224:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD21	1:A:272:ARG:HH11	1.74	0.47
1:B:103:ALA:O	1:B:105:SER:N	2.47	0.47
1:B:429:VAL:HG13	1:B:439:VAL:HG11	1.96	0.47
1:A:3:HIS:O	1:A:6:PRO:HD2	2.14	0.47
1:B:342:ALA:O	1:B:345:ASP:OD2	2.31	0.47
1:B:288:SER:O	1:B:292:VAL:HG22	2.15	0.47
1:A:201:VAL:HG22	1:A:278:PHE:HB2	1.97	0.47
1:A:56:ALA:O	1:A:202:LYS:HG3	2.15	0.46
1:B:131:ARG:HH21	1:B:189:ALA:HB1	1.80	0.46
1:B:387:ALA:HA	1:B:389:HIS:CE1	2.50	0.46
1:A:135:LEU:C	1:A:135:LEU:HD23	2.36	0.46
1:B:191:TYR:O	1:B:194:GLN:HB3	2.16	0.45
1:B:86:GLN:O	1:B:108:PRO:HD2	2.16	0.45
1:A:273:VAL:CG2	1:A:274:GLY:N	2.78	0.45
1:A:422:ARG:NH2	2:A:624:HOH:O	2.47	0.45
1:B:16:LEU:HB2	1:B:39:PHE:HE2	1.82	0.45
1:A:272:ARG:HH21	1:A:308:ASP:HB2	1.75	0.45
1:A:78:ARG:NH2	1:A:127:PRO:HG3	2.31	0.45
1:B:317:VAL:O	1:B:387:ALA:HB3	2.16	0.45
1:B:57:ASP:O	1:B:57:ASP:OD1	2.35	0.44
1:B:405:ARG:NH1	1:B:405:ARG:O	2.51	0.44
1:A:351:ARG:HA	1:A:351:ARG:HD3	1.77	0.44
1:A:272:ARG:HH22	1:A:308:ASP:CG	2.18	0.44
1:A:5:ILE:HB	1:A:6:PRO:HD3	2.00	0.44
1:B:110:ASN:HD21	1:B:112:MET:HB2	1.83	0.44
1:A:315:THR:O	1:A:315:THR:HG22	2.18	0.44
1:B:149:ARG:N	1:B:149:ARG:HD2	2.33	0.44
1:A:433:GLN:O	1:A:436:GLY:N	2.41	0.44
1:A:46:PRO:HD3	1:A:272:ARG:O	2.18	0.43
1:B:8:TYR:O	1:B:11:SER:HB3	2.18	0.43
1:A:81:ALA:O	1:A:85:ARG:HG3	2.18	0.43
1:A:106:HIS:ND1	1:A:177:TYR:HD2	2.17	0.43
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.79	0.43
1:A:55:ASP:HB3	1:A:58:VAL:HG21	1.99	0.43
1:B:46:PRO:HD3	1:B:272:ARG:O	2.18	0.43
1:A:325:ASP:HB2	2:A:679:HOH:O	2.19	0.43
1:A:209:ALA:O	1:A:213:THR:HG23	2.18	0.43
1:B:240:SER:HB3	2:B:475:HOH:O	2.18	0.43
1:B:277:VAL:HG11	1:B:291:GLY:HA2	2.00	0.43
1:A:385:GLY:O	1:A:388:VAL:HG23	2.19	0.43
1:A:131:ARG:HD3	2:A:675:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:NH2	1:B:308:ASP:CB	2.82	0.42
1:B:386:GLY:HA2	2:B:608:HOH:O	2.19	0.42
1:B:142:MET:HE2	1:B:197:VAL:HG11	2.00	0.42
1:A:322:ARG:NH2	1:A:322:ARG:HG2	2.34	0.42
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.85	0.42
1:B:237:MET:CE	1:B:266:LEU:HD13	2.49	0.42
1:B:290:ARG:HD2	2:B:480:HOH:O	2.18	0.42
1:B:202:LYS:HD2	2:B:592:HOH:O	2.20	0.42
1:A:217:HIS:CE1	1:A:219:MET:HG2	2.54	0.42
1:B:4:PRO:O	1:B:7:ASP:HB2	2.20	0.42
1:B:321:GLU:HB2	1:B:328:PHE:HB2	2.02	0.42
1:B:149:ARG:H	1:B:149:ARG:CD	2.32	0.42
1:A:266:LEU:HD22	1:A:267:GLY:N	2.35	0.42
1:A:422:ARG:HB3	1:A:422:ARG:HH11	1.84	0.42
1:B:64:SER:C	1:B:66:SER:H	2.23	0.42
1:A:432:LEU:O	1:A:435:ASP:HB2	2.19	0.41
1:B:188:VAL:O	1:B:192:VAL:HG23	2.21	0.41
1:B:388:VAL:HG12	1:B:388:VAL:O	2.21	0.41
1:A:41:ILE:CA	1:A:201:VAL:HG11	2.49	0.41
1:B:63:GLN:HG3	1:B:261:VAL:HG22	2.02	0.41
1:A:429:VAL:HA	1:A:432:LEU:HD12	2.02	0.41
1:B:122:GLN:HB2	1:B:180:LEU:HD22	2.02	0.41
1:A:389:HIS:HD2	1:A:390:GLU:H	1.69	0.41
1:B:42:ALA:HB2	1:B:201:VAL:HG23	2.03	0.41
1:B:62:ILE:HD12	1:B:142:MET:HE3	2.03	0.41
1:B:323:GLU:HA	1:B:323:GLU:OE1	2.20	0.41
1:A:284:GLU:HG2	1:A:285:VAL:HG13	2.03	0.41
1:B:422:ARG:HB2	2:B:639:HOH:O	2.21	0.41
1:B:410:ASN:HA	1:B:442:GLU:HB2	2.01	0.41
1:A:389:HIS:CD2	1:A:390:GLU:N	2.89	0.41
1:B:91:PRO:HB3	1:B:239:SER:O	2.20	0.41
1:B:135:LEU:HD13	1:B:135:LEU:C	2.42	0.40
1:B:273:VAL:CG2	1:B:274:GLY:N	2.84	0.40
1:B:56:ALA:CA	1:B:201:VAL:HG22	2.51	0.40
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.82	0.40
1:B:315:THR:HG22	1:B:315:THR:O	2.21	0.40
1:A:269:LEU:CD2	1:A:272:ARG:HH11	2.33	0.40
1:A:202:LYS:NZ	2:A:559:HOH:O	2.51	0.40
1:B:335:ILE:O	1:B:417:ILE:HA	2.21	0.40
1:A:110:ASN:HD22	1:A:112:MET:N	2.06	0.40
1:B:56:ALA:HA	1:B:201:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD11	1:A:346:ALA:HB1	2.03	0.40
1:B:418:ASP:O	1:B:422:ARG:HG3	2.21	0.40
1:B:406:THR:HG23	1:B:438:ARG:O	2.21	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	409/456 (90%)	389 (95%)	16 (4%)	4 (1%)	19	21
1	B	405/456 (89%)	380 (94%)	21 (5%)	4 (1%)	19	21
All	All	814/912 (89%)	769 (94%)	37 (4%)	8 (1%)	19	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	ALA
1	B	104	GLU
1	A	106	HIS
1	A	384	GLY
1	B	351	ARG
1	A	324	GLY
1	A	444	PRO
1	B	388	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	313/341 (92%)	307 (98%)	6 (2%)	65 81
1	B	311/341 (91%)	300 (96%)	11 (4%)	43 58
All	All	624/682 (92%)	607 (97%)	17 (3%)	52 70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	250	LEU
1	A	266	LEU
1	A	272	ARG
1	A	284	GLU
1	A	389	HIS
1	B	47	THR
1	B	70	THR
1	B	78	ARG
1	B	149	ARG
1	B	158	GLU
1	B	160	GLU
1	B	248	GLN
1	B	250	LEU
1	B	266	LEU
1	B	272	ARG
1	B	345	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	110	ASN
1	A	121	HIS
1	A	181	GLN
1	A	248	GLN
1	A	389	HIS
1	B	26	GLN
1	B	90	ASN
1	B	110	ASN
1	B	121	HIS
1	B	248	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	415/456 (91%)	1.02	71 (17%) 2 3	19, 33, 75, 110	0
1	B	411/456 (90%)	0.96	69 (16%) 2 3	19, 34, 75, 109	0
All	All	826/912 (90%)	0.99	140 (16%) 2 3	19, 34, 75, 110	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	GLU	9.5
1	B	323	GLU	8.3
1	A	392	ALA	8.1
1	B	392	ALA	7.7
1	A	402	GLY	6.8
1	B	402	GLY	6.7
1	A	379	LEU	6.2
1	B	324	GLY	6.2
1	B	387	ALA	6.2
1	A	382	ALA	6.0
1	B	444	PRO	6.0
1	A	324	GLY	5.9
1	A	406	THR	5.6
1	A	380	SER	5.5
1	A	103	ALA	5.5
1	A	104	GLU	5.5
1	B	103	ALA	5.5
1	A	351	ARG	5.2
1	B	383	THR	5.0
1	A	378	ALA	5.0
1	B	438	ARG	5.0
1	A	377	ALA	5.0
1	A	277	VAL	4.8
1	B	388	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	444	PRO	4.8
1	B	382	ALA	4.7
1	B	102	GLU	4.7
1	B	433	GLN	4.6
1	A	438	ARG	4.6
1	B	437	VAL	4.6
1	B	350	LEU	4.5
1	B	104	GLU	4.5
1	A	437	VAL	4.5
1	B	403	PRO	4.4
1	A	433	GLN	4.4
1	A	353	GLY	4.4
1	A	29	PRO	4.4
1	A	350	LEU	4.1
1	A	393	ALA	4.1
1	B	321	GLU	4.0
1	A	441	VAL	4.0
1	B	384	GLY	3.8
1	B	277	VAL	3.8
1	A	102	GLU	3.8
1	A	403	PRO	3.8
1	B	29	PRO	3.8
1	B	351	ARG	3.7
1	A	105	SER	3.7
1	B	429	VAL	3.6
1	A	321	GLU	3.6
1	A	388	VAL	3.6
1	B	393	ALA	3.6
1	B	381	ALA	3.6
1	B	441	VAL	3.6
1	B	406	THR	3.6
1	A	394	ALA	3.6
1	A	407	VAL	3.6
1	A	322	ARG	3.5
1	B	325	ASP	3.5
1	B	405	ARG	3.5
1	A	442	GLU	3.5
1	A	383	THR	3.4
1	B	57	ASP	3.4
1	A	284	GLU	3.4
1	A	387	ALA	3.3
1	B	426	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	319	PHE	3.3
1	A	279	SER	3.2
1	B	322	ARG	3.2
1	A	404	ILE	3.1
1	A	419	ASP	3.1
1	A	101	LEU	3.1
1	B	389	HIS	3.1
1	A	319	PHE	3.0
1	A	391	ALA	3.0
1	B	407	VAL	2.9
1	A	265	VAL	2.9
1	A	320	VAL	2.9
1	B	353	GLY	2.9
1	B	118	LEU	2.9
1	B	105	SER	2.9
1	B	425	ILE	2.8
1	B	124	LEU	2.8
1	B	320	VAL	2.8
1	B	404	ILE	2.8
1	B	445	GLU	2.8
1	A	325	ASP	2.8
1	B	432	LEU	2.7
1	B	394	ALA	2.7
1	B	128	GLU	2.7
1	B	347	LEU	2.7
1	A	381	ALA	2.7
1	B	279	SER	2.6
1	B	101	LEU	2.6
1	B	409	LEU	2.6
1	A	162	ALA	2.6
1	B	284	GLU	2.6
1	B	162	ALA	2.6
1	B	436	GLY	2.6
1	A	429	VAL	2.6
1	A	384	GLY	2.5
1	A	426	ALA	2.5
1	A	409	LEU	2.5
1	B	411	LEU	2.5
1	A	149	ARG	2.5
1	B	250	LEU	2.5
1	A	106	HIS	2.5
1	A	417	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	280	PRO	2.5
1	A	39	PHE	2.4
1	B	440	GLU	2.4
1	B	149	ARG	2.4
1	A	425	ILE	2.4
1	B	419	ASP	2.4
1	A	250	LEU	2.3
1	B	106	HIS	2.3
1	B	174	LEU	2.3
1	A	411	LEU	2.3
1	A	278	PHE	2.3
1	B	285	VAL	2.3
1	A	436	GLY	2.2
1	A	405	ARG	2.2
1	A	329	LEU	2.2
1	A	445	GLU	2.2
1	A	85	ARG	2.2
1	A	57	ASP	2.2
1	B	129	ALA	2.2
1	A	158	GLU	2.2
1	A	14	THR	2.2
1	A	10	ALA	2.2
1	A	124	LEU	2.2
1	A	255	ILE	2.1
1	B	412	ALA	2.1
1	B	220	THR	2.1
1	A	280	PRO	2.1
1	B	265	VAL	2.1
1	B	422	ARG	2.0
1	A	352	THR	2.0
1	B	442	GLU	2.0
1	B	35	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.