Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 12:41 PM EST

PDB ID	:	4P22
Title	:	Crystal Structure of N-terminal Fragments of E1
Authors	:	Xie, S.-T.
Deposited on	:	2014-02-28
Resolution	:	2.75 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:

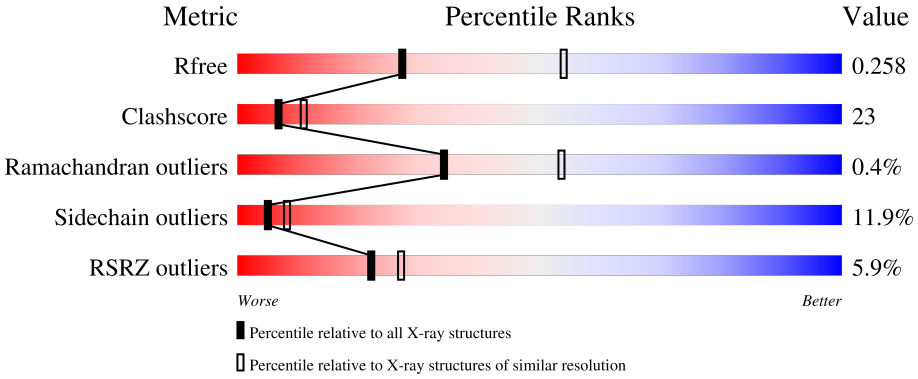
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	446	6% 52% 28% • 17%
1	B	446	4% 58% 21% 5% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5848 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 Ubiquitin-like modifier-activating enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2851	1812	487	537	15	0	0	0
1	B	375	2888	1834	492	546	16	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P22314
A	-5	PRO	-	expression tag	UNP P22314
A	-4	HIS	-	expression tag	UNP P22314
A	-3	MET	-	expression tag	UNP P22314
A	-2	ALA	-	expression tag	UNP P22314
A	-1	ASP	-	expression tag	UNP P22314
A	0	LEU	-	expression tag	UNP P22314
A	352	ASP	GLU	engineered mutation	UNP P22314
B	-6	GLY	-	expression tag	UNP P22314
B	-5	PRO	-	expression tag	UNP P22314
B	-4	HIS	-	expression tag	UNP P22314
B	-3	MET	-	expression tag	UNP P22314
B	-2	ALA	-	expression tag	UNP P22314
B	-1	ASP	-	expression tag	UNP P22314
B	0	LEU	-	expression tag	UNP P22314
B	352	ASP	GLU	engineered mutation	UNP P22314

- Molecule 2 is water.

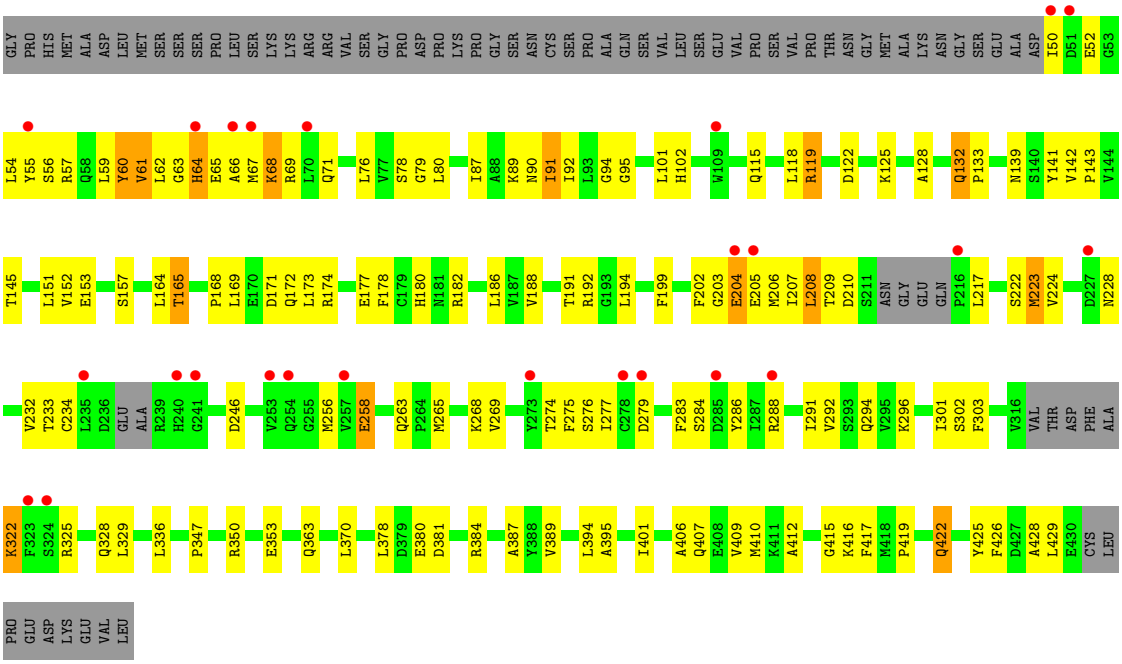
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	44	44	44	0	0
2	B	65	65	65	0	0

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.

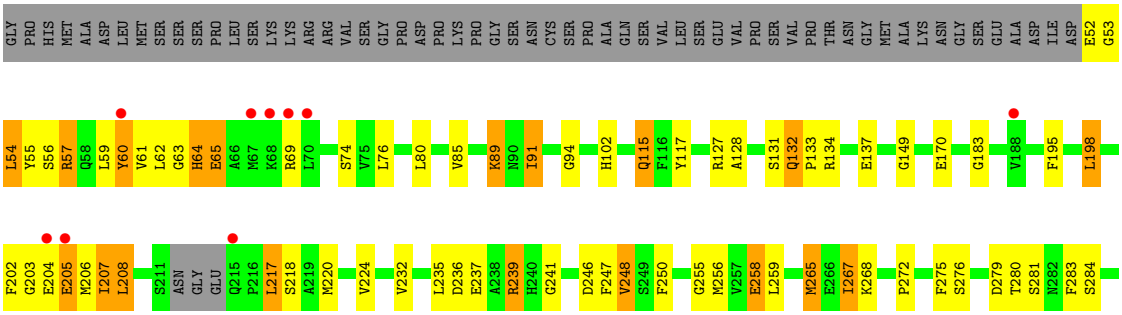
• Molecule 1: Ubiquitin-like modifier-activating enzyme 1

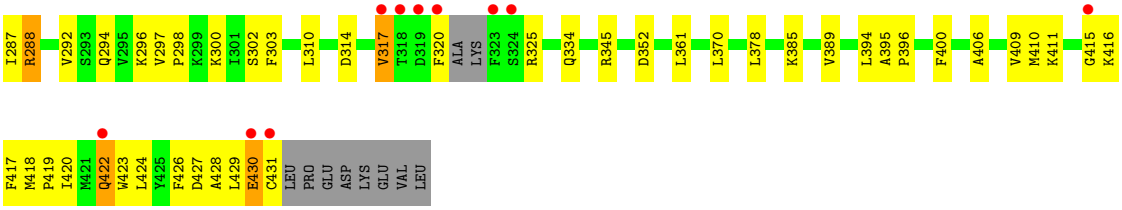
Chain A: 6% 52% 28% • 17%



• Molecule 1: Ubiquitin-like modifier-activating enzyme 1

Chain B: 4% 58% 21% 5% 16%




I287
R288
V292
S293
Q294
V295
K296
V297
P298
K299
K300
I301
S302
F303
L310
D314
V317
T318
D319
F320
ALA
LYS
F323
S324
R325
Q334
R345
D352
L361
L370
L378
K385
V389
L394
A395
P396
F400
A406
V409
M410
K411
G415
K416
F417
M418
P419
I420
M421
Q422
W423
L424
Y425
F426
D427
A428
L429
E430
C431
LEU
PRO
GLU
ASP
LYS
GLU
VAL
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	94.13Å 186.81Å 135.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.75 29.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.77-2.75) 98.3 (29.77-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.264 0.210 , 0.258	Depositor DCC
R_{free} test set	1559 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.45	1/2904 (0.0%)	0.63	0/3929
1	B	0.42	0/2943	0.63	0/3986
All	All	0.43	1/5847 (0.0%)	0.63	0/7915

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	TYR	CB-CG	-5.16	1.44	1.51

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	2851	0	2835	136	0
1	B	2888	0	2860	167	0
2	A	44	0	0	0	0
2	B	65	0	0	3	0
All	All	5848	0	5695	266	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 23.

All (266) 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:80:LEU:CD2	1:B:128:ALA:HA	1.37	1.52
1:A:389:VAL:HG22	1:B:60:TYR:CE1	1.55	1.40
1:A:389:VAL:HG22	1:B:60:TYR:CZ	1.69	1.25
1:A:64:HIS:NE2	1:B:394:LEU:HA	1.57	1.19
1:B:80:LEU:HD22	1:B:128:ALA:CA	1.75	1.15
1:A:68:LYS:HD2	1:A:68:LYS:O	1.46	1.13
1:B:57:ARG:HA	1:B:60:TYR:CD2	1.89	1.07
1:B:207:ILE:HD11	1:B:416:LYS:HE3	1.25	1.07
1:B:422:GLN:HE21	1:B:422:GLN:CA	1.59	1.06
1:B:422:GLN:HA	1:B:422:GLN:NE2	1.58	1.06
1:B:80:LEU:CD2	1:B:128:ALA:CA	2.33	1.04
1:A:389:VAL:CG2	1:B:60:TYR:CE1	2.40	1.03
1:B:428:ALA:O	1:B:429:LEU:HD12	1.58	1.03
1:B:80:LEU:HD22	1:B:128:ALA:HA	1.03	1.00
1:B:422:GLN:HG3	2:B:524:HOH:O	1.57	1.00
1:B:207:ILE:CD1	1:B:416:LYS:HE3	1.92	0.98
1:B:80:LEU:HD23	1:B:128:ALA:HA	1.41	0.98
1:B:62:LEU:HD22	1:B:417:PHE:HD2	1.27	0.96
1:B:314:ASP:O	1:B:422:GLN:HB2	1.65	0.94
1:A:429:LEU:HD13	1:B:59:LEU:HD22	1.50	0.93
1:B:62:LEU:HD22	1:B:417:PHE:CD2	2.04	0.93
1:B:428:ALA:C	1:B:429:LEU:HD12	1.88	0.93
1:A:389:VAL:HG22	1:B:60:TYR:OH	1.68	0.91
1:A:91:ILE:HD11	1:A:409:VAL:HG11	1.49	0.91
1:B:57:ARG:HA	1:B:60:TYR:CE2	2.05	0.90
1:A:268:LYS:HB3	1:A:276:SER:OG	1.71	0.90
1:A:394:LEU:HA	1:B:64:HIS:NE2	1.86	0.88
1:B:422:GLN:HE21	1:B:422:GLN:HA	0.74	0.88
1:B:427:ASP:OD2	1:B:429:LEU:HD13	1.74	0.88
1:B:56:SER:O	1:B:60:TYR:CE1	2.27	0.88
1:B:64:HIS:HB2	1:B:94:GLY:O	1.74	0.88
1:A:389:VAL:HG22	1:B:60:TYR:HE1	1.29	0.86
1:A:52:GLU:HG2	1:A:279:ASP:OD1	1.77	0.84
1:A:80:LEU:HD11	1:A:101:LEU:HB3	1.60	0.82
1:A:389:VAL:CG2	1:B:60:TYR:OH	2.28	0.82
1:A:60:TYR:OH	1:B:389:VAL:HG22	1.81	0.80
1:A:199:PHE:HA	1:A:422:GLN:O	1.80	0.80
1:B:62:LEU:CD2	1:B:417:PHE:HD2	1.94	0.80
1:A:68:LYS:O	1:A:68:LYS:CD	2.30	0.79
1:B:63:GLY:O	1:B:64:HIS:CD2	2.35	0.79
1:A:389:VAL:CG2	1:B:60:TYR:HE1	1.84	0.78
1:A:64:HIS:CD2	1:B:394:LEU:HA	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD23	1:B:417:PHE:CZ	2.20	0.77
1:A:429:LEU:CD1	1:B:59:LEU:HD22	2.15	0.76
1:A:381:ASP:OD1	1:A:384:ARG:NH2	2.21	0.74
1:B:63:GLY:O	1:B:64:HIS:CB	2.35	0.74
1:B:63:GLY:O	1:B:64:HIS:HB3	1.87	0.73
1:B:258:GLU:HG3	1:B:283:PHE:CG	2.24	0.72
1:A:122:ASP:HA	1:A:125:LYS:HD2	1.72	0.72
1:A:64:HIS:HB2	1:A:94:GLY:HA2	1.72	0.71
1:A:303:PHE:HZ	1:A:419:PRO:HG2	1.54	0.71
1:A:363:GLN:NE2	1:A:380:GLU:OE2	2.24	0.70
1:B:207:ILE:HB	1:B:300:LYS:HE3	1.73	0.70
1:B:80:LEU:HD22	1:B:128:ALA:CB	2.22	0.70
1:B:246:ASP:OD2	1:B:294:GLN:NE2	2.25	0.69
1:B:61:VAL:HG13	1:B:69:ARG:HD2	1.73	0.69
1:B:56:SER:O	1:B:60:TYR:CZ	2.46	0.69
1:B:422:GLN:CA	1:B:422:GLN:NE2	2.30	0.68
1:B:56:SER:C	1:B:60:TYR:CZ	2.67	0.68
1:B:56:SER:O	1:B:60:TYR:CD1	2.46	0.68
1:A:429:LEU:HD13	1:B:59:LEU:CD2	2.21	0.67
1:A:60:TYR:CZ	1:B:389:VAL:HG22	2.29	0.67
1:A:132:GLN:HG3	1:A:133:PRO:HD3	1.77	0.66
1:A:63:GLY:O	1:A:64:HIS:CD2	2.48	0.66
1:B:62:LEU:CD2	1:B:417:PHE:CD2	2.75	0.66
1:A:325:ARG:HG3	1:A:328:GLN:HG3	1.78	0.66
1:B:430:GLU:C	1:B:430:GLU:OE1	2.35	0.66
1:A:60:TYR:CE2	1:B:389:VAL:HA	2.30	0.65
1:A:246:ASP:OD2	1:A:294:GLN:NE2	2.29	0.65
1:B:427:ASP:OD2	1:B:428:ALA:N	2.30	0.65
1:A:395:ALA:N	1:B:64:HIS:NE2	2.45	0.64
1:B:204:GLU:HA	1:B:302:SER:HA	1.80	0.64
1:B:57:ARG:CA	1:B:60:TYR:CE2	2.81	0.63
1:A:63:GLY:O	1:A:64:HIS:HD2	1.81	0.63
1:A:139:ASN:HB2	1:A:141:TYR:CE1	2.35	0.62
1:B:117:TYR:CE2	1:B:134:ARG:HB3	2.35	0.62
1:B:85:VAL:HG11	1:B:115:GLN:HA	1.80	0.62
1:A:325:ARG:HG2	1:A:328:GLN:HE21	1.66	0.61
1:B:208:LEU:HA	1:B:416:LYS:O	2.01	0.61
1:B:63:GLY:O	1:B:64:HIS:CG	2.54	0.60
1:B:64:HIS:CG	1:B:94:GLY:HA2	2.36	0.60
1:B:250:PHE:HE1	1:B:265:MET:HE1	1.67	0.60
1:B:207:ILE:HD11	1:B:416:LYS:CE	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:LYS:O	1:B:415:GLY:N	2.35	0.59
1:B:56:SER:HB3	1:B:60:TYR:OH	2.02	0.58
1:A:275:PHE:HE1	1:A:277:ILE:CG2	2.15	0.58
1:B:63:GLY:O	1:B:64:HIS:HD2	1.83	0.57
1:B:303:PHE:HZ	1:B:419:PRO:HG2	1.69	0.57
1:A:64:HIS:HB2	1:A:94:GLY:CA	2.33	0.57
1:B:198:LEU:HD12	1:B:420:ILE:HD12	1.86	0.57
1:B:279:ASP:C	1:B:279:ASP:OD2	2.43	0.57
1:A:60:TYR:HE2	1:B:389:VAL:HA	1.69	0.57
1:B:258:GLU:HG3	1:B:283:PHE:CD2	2.40	0.56
1:A:62:LEU:HD12	1:A:415:GLY:HA3	1.87	0.56
1:A:153:GLU:HB2	1:A:178:PHE:CE1	2.40	0.56
1:A:350:ARG:HG3	1:B:57:ARG:HD3	1.87	0.55
1:A:60:TYR:OH	1:B:389:VAL:CG2	2.53	0.55
1:B:303:PHE:CZ	1:B:419:PRO:HG2	2.42	0.55
1:A:233:THR:HG22	1:A:274:THR:HG22	1.89	0.55
1:B:115:GLN:C	1:B:115:GLN:OE1	2.45	0.55
1:A:60:TYR:OH	1:B:389:VAL:HG13	2.07	0.54
1:A:268:LYS:HB3	1:A:276:SER:HG	1.72	0.54
1:B:420:ILE:HG22	1:B:422:GLN:O	2.07	0.54
1:A:64:HIS:NE2	1:B:394:LEU:CA	2.50	0.54
1:A:204:GLU:HA	1:A:303:PHE:H	1.73	0.54
1:A:394:LEU:CA	1:B:64:HIS:NE2	2.66	0.54
1:A:169:LEU:O	1:A:173:LEU:HG	2.09	0.53
1:A:350:ARG:NH2	1:B:53:GLY:HA2	2.23	0.53
1:A:192:ARG:HD3	1:A:336:LEU:HD23	1.90	0.53
1:B:385:LYS:O	1:B:389:VAL:HB	2.08	0.53
1:B:62:LEU:HD11	1:B:411:LYS:HA	1.91	0.53
1:A:50:ILE:HG22	1:A:52:GLU:H	1.73	0.53
1:B:64:HIS:CB	1:B:94:GLY:HA2	2.38	0.53
1:A:322:LYS:HD3	1:B:317:VAL:HG22	1.91	0.52
1:B:115:GLN:NE2	1:B:131:SER:OG	2.42	0.52
1:A:171:ASP:OD2	1:A:174:ARG:NH2	2.43	0.52
1:A:207:ILE:O	1:A:416:LYS:HB3	2.08	0.52
1:B:279:ASP:OD2	1:B:280:THR:N	2.42	0.52
1:A:407:GLN:HG2	1:B:396:PRO:HB2	1.92	0.52
1:B:115:GLN:OE1	1:B:115:GLN:CA	2.57	0.52
1:B:207:ILE:HG13	1:B:300:LYS:HZ2	1.73	0.52
1:A:68:LYS:HD2	1:A:68:LYS:C	2.26	0.52
1:A:286:TYR:OH	1:A:288:ARG:O	2.25	0.52
1:B:207:ILE:CD1	1:B:416:LYS:CE	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:HG22	1:B:288:ARG:HD2	1.91	0.52
1:B:411:LYS:O	1:B:415:GLY:HA3	2.09	0.52
1:A:258:GLU:HG3	1:A:283:PHE:CD2	2.45	0.52
1:A:223:MET:HA	1:A:286:TYR:CE2	2.45	0.52
1:B:132:GLN:HG3	1:B:133:PRO:HD3	1.90	0.52
1:B:267:ILE:HG13	1:B:275:PHE:CD1	2.45	0.52
1:B:64:HIS:HB2	1:B:94:GLY:HA2	1.92	0.51
1:A:199:PHE:CE1	1:A:422:GLN:HB3	2.45	0.51
1:A:164:LEU:HB2	1:A:188:VAL:HG22	1.92	0.51
1:B:208:LEU:HD13	1:B:418:MET:HG2	1.91	0.51
1:A:303:PHE:CZ	1:A:419:PRO:HG2	2.42	0.51
1:B:279:ASP:OD2	1:B:281:SER:OG	2.28	0.51
1:B:422:GLN:HB3	1:B:423:TRP:CD1	2.46	0.51
1:B:256:MET:HG3	1:B:283:PHE:HB3	1.92	0.50
1:B:314:ASP:HB2	1:B:422:GLN:HG2	1.93	0.50
1:A:64:HIS:CD2	1:B:394:LEU:CA	2.94	0.50
1:A:256:MET:HB3	1:A:284:SER:O	2.11	0.50
1:A:279:ASP:O	1:A:279:ASP:OD2	2.30	0.50
1:A:208:LEU:HD23	1:A:301:ILE:HB	1.94	0.50
1:B:195:PHE:CD1	1:B:389:VAL:HG11	2.46	0.50
1:A:60:TYR:OH	1:B:389:VAL:CB	2.59	0.50
1:B:423:TRP:CD1	1:B:423:TRP:N	2.79	0.50
1:B:426:PHE:CZ	1:B:428:ALA:HA	2.47	0.49
1:A:194:LEU:HD13	1:A:389:VAL:CG1	2.43	0.49
1:A:217:LEU:H	1:A:217:LEU:HD23	1.78	0.49
1:A:417:PHE:O	1:A:419:PRO:HD3	2.12	0.49
1:A:329:LEU:HD12	1:A:425:TYR:HB3	1.94	0.49
1:B:59:LEU:HD23	1:B:417:PHE:CE1	2.48	0.49
1:A:419:PRO:O	1:B:430:GLU:OE2	2.30	0.49
1:B:280:THR:HG22	1:B:283:PHE:CD1	2.48	0.49
1:B:64:HIS:HB2	1:B:94:GLY:C	2.32	0.48
1:B:224:VAL:HG22	1:B:232:VAL:HG22	1.95	0.48
1:A:54:LEU:HB3	1:A:263:GLN:HB2	1.95	0.48
1:B:422:GLN:HB3	1:B:423:TRP:HD1	1.78	0.48
1:B:248:VAL:HG13	1:B:292:VAL:HG23	1.95	0.48
1:B:60:TYR:O	1:B:65:GLU:HB3	2.13	0.48
1:B:239:ARG:HD2	1:B:272:PRO:O	2.12	0.48
1:B:411:LYS:O	1:B:415:GLY:CA	2.62	0.48
1:A:222:SER:HB2	1:A:234:CYS:HA	1.96	0.48
1:A:389:VAL:CG2	1:B:60:TYR:CZ	2.64	0.48
1:B:80:LEU:HD23	1:B:131:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:CD	1:A:118:LEU:HD13	2.34	0.47
1:A:80:LEU:CD1	1:A:101:LEU:HB3	2.37	0.47
1:A:325:ARG:CG	1:A:328:GLN:HG3	2.43	0.47
1:B:132:GLN:HG3	1:B:133:PRO:CD	2.44	0.47
1:B:208:LEU:CA	1:B:416:LYS:O	2.62	0.47
1:A:56:SER:HA	1:A:59:LEU:HD12	1.96	0.47
1:B:94:GLY:HA3	1:B:410:MET:HE1	1.97	0.47
1:B:64:HIS:HB2	1:B:94:GLY:CA	2.44	0.47
1:A:60:TYR:OH	1:B:389:VAL:CA	2.62	0.47
1:A:199:PHE:CD1	1:A:422:GLN:O	2.68	0.47
1:B:94:GLY:HA3	1:B:410:MET:CE	2.44	0.47
1:B:57:ARG:N	1:B:60:TYR:CE2	2.82	0.46
1:A:92:ILE:O	1:A:139:ASN:ND2	2.48	0.46
1:A:55:TYR:CE1	1:A:417:PHE:HE1	2.33	0.46
1:A:87:ILE:O	1:A:91:ILE:HB	2.16	0.46
1:B:430:GLU:OE1	1:B:430:GLU:O	2.32	0.46
1:B:56:SER:CB	1:B:60:TYR:OH	2.63	0.46
1:A:80:LEU:HD13	1:A:128:ALA:HA	1.98	0.46
1:A:192:ARG:HD3	1:A:336:LEU:CD2	2.46	0.46
1:A:204:GLU:HG2	1:A:303:PHE:O	2.16	0.46
1:A:64:HIS:CB	1:A:94:GLY:HA2	2.43	0.46
1:A:79:GLY:HA3	1:A:165:THR:HG22	1.97	0.46
1:B:352:ASP:N	1:B:352:ASP:OD2	2.49	0.46
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.69	0.45
1:A:64:HIS:HB2	1:A:94:GLY:O	2.16	0.45
1:A:78:SER:O	1:A:165:THR:HB	2.17	0.45
1:B:406:ALA:O	1:B:410:MET:HG2	2.16	0.45
1:A:61:VAL:HG22	1:A:66:ALA:HB3	1.98	0.45
1:A:275:PHE:CE1	1:A:277:ILE:CG2	2.98	0.45
1:A:389:VAL:HG23	1:B:60:TYR:OH	2.14	0.45
1:A:50:ILE:HG22	1:A:52:GLU:N	2.32	0.45
1:B:255:GLY:O	1:B:284:SER:HB2	2.16	0.45
1:A:61:VAL:HG11	1:A:69:ARG:NH2	2.32	0.45
1:A:60:TYR:O	1:A:65:GLU:HB3	2.17	0.44
1:A:89:LYS:HE3	1:A:90:ASN:OD1	2.16	0.44
1:A:203:GLY:O	1:A:205:GLU:N	2.49	0.44
1:B:59:LEU:CD2	1:B:417:PHE:CE1	3.00	0.44
1:B:280:THR:HG22	1:B:283:PHE:CE1	2.52	0.44
1:A:224:VAL:HG12	1:A:286:TYR:CD1	2.53	0.44
1:B:89:LYS:HE3	1:B:89:LYS:HB3	1.66	0.44
1:B:325:ARG:H	1:B:325:ARG:HG3	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:CZ	1:A:182:ARG:HD3	2.53	0.44
1:B:91:ILE:HD11	1:B:409:VAL:HB	1.99	0.44
1:A:64:HIS:HD2	1:B:394:LEU:HB3	1.82	0.44
1:A:102:HIS:CG	1:A:151:LEU:HD21	2.53	0.44
1:A:141:TYR:CD2	1:A:142:VAL:HG23	2.52	0.44
1:A:406:ALA:O	1:A:410:MET:HG2	2.18	0.44
1:B:102:HIS:NE2	1:B:149:GLY:O	2.48	0.44
1:B:69:ARG:HB2	2:B:543:HOH:O	2.17	0.43
1:A:322:LYS:HB3	1:A:322:LYS:HE2	1.80	0.43
1:A:60:TYR:HB3	1:A:65:GLU:HG2	1.99	0.43
1:B:60:TYR:CD1	1:B:60:TYR:N	2.84	0.43
1:B:54:LEU:H	1:B:54:LEU:HD22	1.82	0.43
1:B:250:PHE:CE1	1:B:265:MET:HE1	2.50	0.43
1:B:268:LYS:HB3	1:B:276:SER:OG	2.18	0.43
1:A:202:PHE:CE2	1:A:419:PRO:HB3	2.54	0.43
1:A:203:GLY:C	1:A:205:GLU:H	2.22	0.43
1:A:232:VAL:HG21	1:A:275:PHE:CE1	2.54	0.43
1:B:297:VAL:HA	1:B:298:PRO:HD3	1.86	0.43
1:A:69:ARG:O	1:A:71:GLN:HG2	2.17	0.43
1:A:325:ARG:CG	1:A:328:GLN:HE21	2.31	0.43
1:B:80:LEU:HD23	1:B:127:ARG:O	2.18	0.43
1:A:57:ARG:HB2	1:A:263:GLN:HE22	1.83	0.42
1:A:64:HIS:NE2	1:B:395:ALA:N	2.66	0.42
1:A:153:GLU:HB2	1:A:178:PHE:CZ	2.54	0.42
1:A:178:PHE:CE1	1:A:182:ARG:HD3	2.54	0.42
1:B:206:MET:HB2	1:B:206:MET:HE2	1.91	0.42
1:B:207:ILE:HB	1:B:300:LYS:CE	2.46	0.42
1:A:54:LEU:HD22	1:A:265:MET:HG2	2.01	0.42
1:B:64:HIS:O	1:B:64:HIS:ND1	2.52	0.42
1:B:203:GLY:C	1:B:205:GLU:H	2.23	0.42
1:A:202:PHE:CZ	1:A:412:ALA:HB2	2.55	0.42
1:A:177:GLU:HG3	1:A:178:PHE:N	2.35	0.42
1:B:80:LEU:HD23	1:B:128:ALA:CA	2.29	0.42
1:B:195:PHE:HD1	1:B:389:VAL:HG11	1.84	0.42
1:A:119:ARG:HH12	1:B:137:GLU:HB3	1.85	0.42
1:B:55:TYR:HB2	1:B:247:PHE:CD2	2.54	0.42
1:B:426:PHE:CE1	1:B:427:ASP:O	2.73	0.42
1:A:95:GLY:HA2	1:A:142:VAL:HG21	2.02	0.42
1:A:426:PHE:CZ	1:A:428:ALA:HA	2.55	0.42
1:B:427:ASP:OD2	1:B:427:ASP:C	2.57	0.41
1:B:428:ALA:C	1:B:429:LEU:CD1	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:CD1	1:A:415:GLY:HA3	2.49	0.41
1:A:232:VAL:HG23	1:A:277:ILE:HG23	2.02	0.41
1:B:183:GLY:HA2	2:B:559:HOH:O	2.20	0.41
1:B:208:LEU:CB	1:B:416:LYS:O	2.69	0.41
1:A:65:GLU:HG3	1:A:66:ALA:N	2.35	0.41
1:A:142:VAL:HA	1:A:143:PRO:HD3	1.92	0.41
1:B:265:MET:HE3	1:B:265:MET:HB2	1.70	0.41
1:A:63:GLY:O	1:B:394:LEU:HD22	2.20	0.41
1:B:56:SER:C	1:B:60:TYR:CE2	2.94	0.41
1:A:168:PRO:O	1:A:172:GLN:HG3	2.21	0.40
1:A:61:VAL:CG1	1:A:69:ARG:NE	2.84	0.40
1:B:202:PHE:CE2	1:B:419:PRO:HB3	2.56	0.40
1:A:180:HIS:NE2	1:A:204:GLU:HG3	2.35	0.40
1:A:347:PRO:HB2	1:A:387:ALA:O	2.21	0.40
1:B:205:GLU:H	1:B:205:GLU:HG3	1.65	0.40
1:B:314:ASP:O	1:B:422:GLN:CB	2.53	0.40
1:A:350:ARG:CG	1:B:57:ARG:HD3	2.52	0.40
1:A:66:ALA:O	1:A:69:ARG:HD3	2.22	0.40
1:B:217:LEU:HD11	1:B:241:GLY:HA3	2.02	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	362/446 (81%)	341 (94%)	20 (6%)	1 (0%)	41	60
1	B	369/446 (83%)	352 (95%)	15 (4%)	2 (0%)	29	47
All	All	731/892 (82%)	693 (95%)	35 (5%)	3 (0%)	34	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	A	204	GLU
1	B	317	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	308/372 (83%)	276 (90%)	32 (10%)	7 11
1	B	312/372 (84%)	270 (86%)	42 (14%)	4 5
All	All	620/744 (83%)	546 (88%)	74 (12%)	5 8

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	64	HIS
1	A	67	MET
1	A	68	LYS
1	A	76	LEU
1	A	91	ILE
1	A	119	ARG
1	A	132	GLN
1	A	145	THR
1	A	152	VAL
1	A	157	SER
1	A	165	THR
1	A	186	LEU
1	A	191	THR
1	A	206	MET
1	A	208	LEU
1	A	209	THR
1	A	210	ASP
1	A	223	MET
1	A	228	ASN
1	A	258	GLU

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Mol	Chain	Res	Type
1	A	269	VAL
1	A	291	ILE
1	A	292	VAL
1	A	296	LYS
1	A	302	SER
1	A	322	LYS
1	A	353	GLU
1	A	370	LEU
1	A	378	LEU
1	A	401	ILE
1	A	422	GLN
1	B	52	GLU
1	B	54	LEU
1	B	57	ARG
1	B	60	TYR
1	B	65	GLU
1	B	74	SER
1	B	76	LEU
1	B	89	LYS
1	B	91	ILE
1	B	115	GLN
1	B	132	GLN
1	B	170	GLU
1	B	198	LEU
1	B	205	GLU
1	B	207	ILE
1	B	208	LEU
1	B	217	LEU
1	B	218	SER
1	B	220	MET
1	B	235	LEU
1	B	236	ASP
1	B	237	GLU
1	B	239	ARG
1	B	248	VAL
1	B	258	GLU
1	B	259	LEU
1	B	265	MET
1	B	267	ILE
1	B	288	ARG
1	B	296	LYS
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	320	PHE
1	B	334	GLN
1	B	345	ARG
1	B	361	LEU
1	B	370	LEU
1	B	378	LEU
1	B	400	PHE
1	B	422	GLN
1	B	424	LEU
1	B	430	GLU
1	B	431	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	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	370/446 (82%)	0.13	25 (6%)	17	20	16, 41, 107, 152	0
1	B	375/446 (84%)	-0.12	19 (5%)	28	34	15, 36, 78, 135	0
All	All	745/892 (83%)	0.00	44 (5%)	22	27	15, 38, 100, 152	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	5.8
1	A	216	PRO	5.6
1	B	60	TYR	5.1
1	B	318	THR	4.7
1	A	66	ALA	4.1
1	B	204	GLU	4.1
1	A	324	SER	4.1
1	B	319	ASP	4.0
1	A	288	ARG	3.9
1	B	323	PHE	3.8
1	A	51	ASP	3.7
1	A	273	TYR	3.5
1	A	257	VAL	3.5
1	B	67	MET	3.4
1	A	67	MET	3.0
1	B	430	GLU	3.0
1	A	227	ASP	2.9
1	B	317	VAL	2.8
1	A	109	TRP	2.8
1	A	278	CYS	2.7
1	A	235	LEU	2.7
1	A	253	VAL	2.7
1	A	254	GLN	2.7
1	A	279	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	241	GLY	2.7
1	B	205	GLU	2.6
1	B	215	GLN	2.6
1	B	431	CYS	2.6
1	A	240	HIS	2.6
1	A	323	PHE	2.6
1	A	285	ASP	2.5
1	B	415	GLY	2.4
1	B	422	GLN	2.4
1	B	70	LEU	2.3
1	B	324	SER	2.3
1	A	50	ILE	2.3
1	B	320	PHE	2.2
1	A	70	LEU	2.2
1	A	55	TYR	2.2
1	B	188	VAL	2.2
1	B	69	ARG	2.2
1	A	205	GLU	2.1
1	B	68	LYS	2.1
1	A	64	HIS	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.