Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 09:34 AM EDT

PDB ID	:	5EJJ
Title	:	Crystal structure of UfSP from C.elegans
Authors	:	Kim, K.; Ha, B.; Kim, E.E.
Deposited on	:	2015-11-02
Resolution	:	2.80 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:

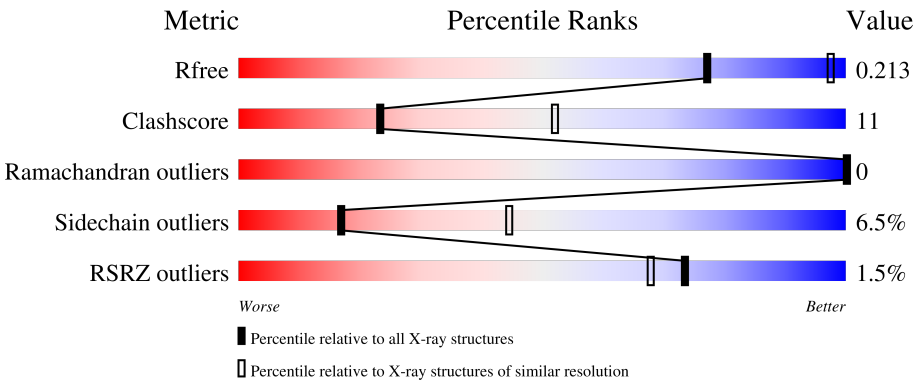
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	564	2% 68% 21% • 8%
1	B	564	% 64% 26% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8530 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 Ufm1-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4138	2626	724	771	17	0	0	0
1	B	520	4169	2650	727	775	17	0	0	0

- Molecule 2 is water.

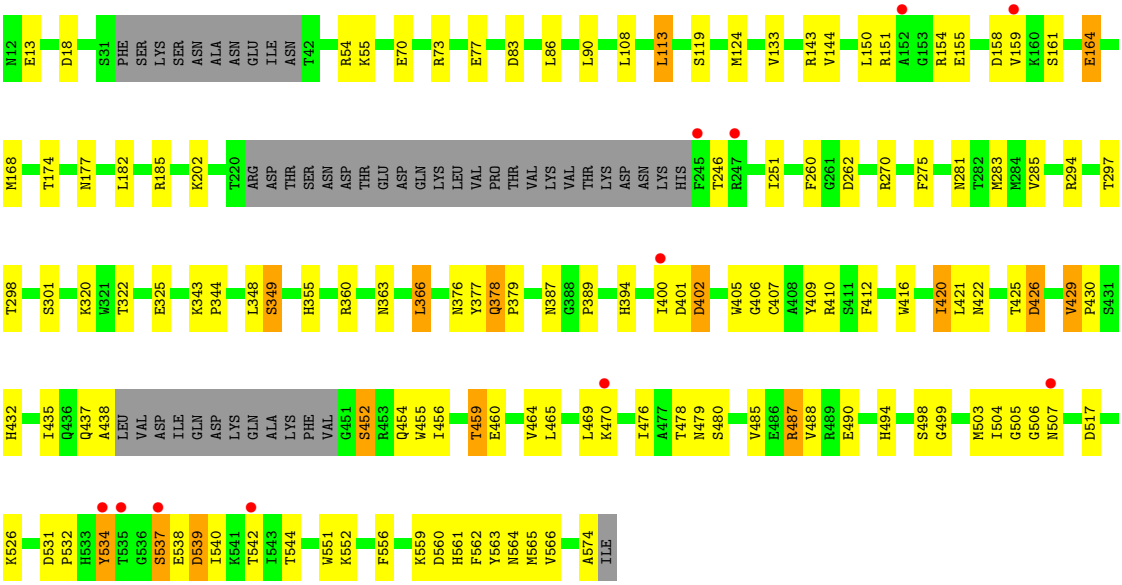
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	108	108	108	0	0
2	B	115	115	115	0	0

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.

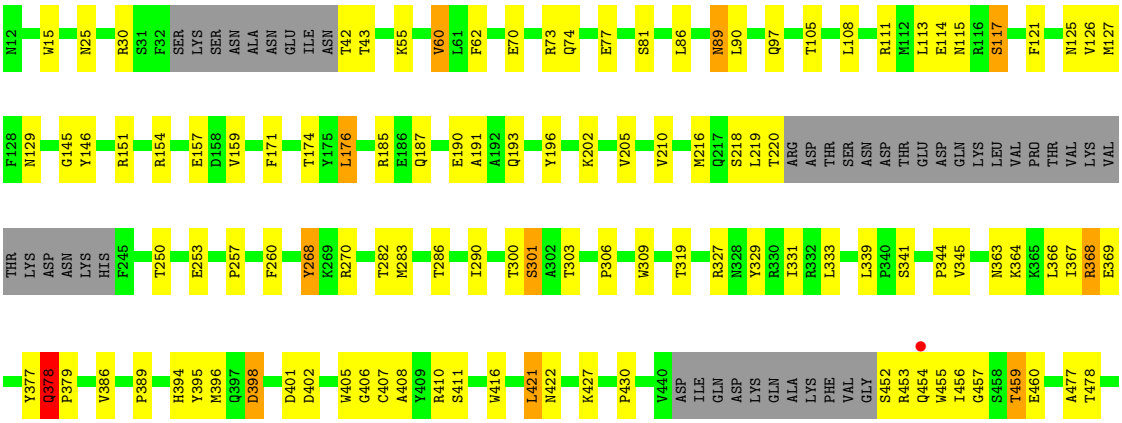
- Molecule 1: Ufm1-specific protease

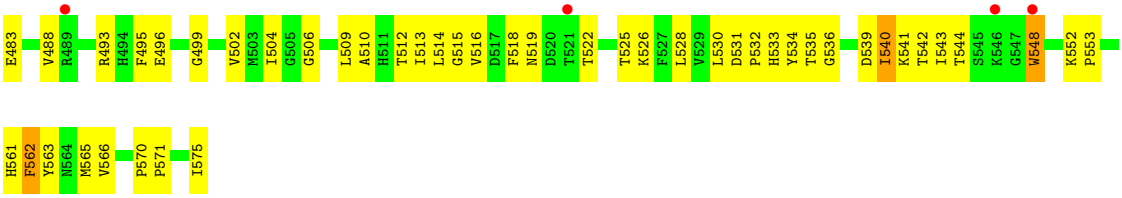
Chain A: 2% 68% 21% 8%



- Molecule 1: Ufm1-specific protease

Chain B: % 64% 26% 8%




E483
V488
R489
R493
H494
F495
E496
G499
V502
M503
I504
G505
G506
L509
A510
H511
T512
I513
L514
G515
V516
D517
F518
N519
D520
T521
T522
T525
K526
F527
L528
V529
L530
D531
P532
H533
Y534
T535
G536
D539
I540
K541
T542
I543
T544
S545
K546
G547
W548
K552
P553

H561
F562
Y563
N564
M565
V566
P570
P571
I575

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.53Å 149.81Å 226.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.28 – 2.80 41.28 – 2.79	Depositor EDS
% Data completeness (in resolution range)	91.6 (41.28-2.80) 93.8 (41.28-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.206 , 0.237 0.214 , 0.213	Depositor DCC
R_{free} test set	3161 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8530	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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	0.52	0/4235	0.72	5/5736 (0.1%)
1	B	0.49	0/4267	0.68	5/5779 (0.1%)
All	All	0.51	0/8502	0.70	10/11515 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	438	ALA	N-CA-CB	15.93	132.41	110.10
1	B	378	GLN	CB-CA-C	-8.44	93.53	110.40
1	B	535	THR	N-CA-CB	7.01	123.63	110.30
1	A	538	GLU	N-CA-C	-6.93	92.30	111.00
1	B	378	GLN	N-CA-C	6.87	129.54	111.00
1	A	539	ASP	N-CA-C	-6.63	93.09	111.00
1	A	437	GLN	N-CA-C	-5.73	95.54	111.00
1	B	368	ARG	CB-CA-C	5.64	121.68	110.40
1	B	89	ASN	CB-CA-C	-5.39	99.61	110.40
1	A	539	ASP	N-CA-CB	5.00	119.60	110.60

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	4138	0	4047	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4169	0	4084	105	0
2	A	108	0	0	5	0
2	B	115	0	0	8	0
All	All	8530	0	8131	185	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 11.

All (185) 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:262:ASP:OD1	1:A:270:ARG:NH2	2.08	0.86
1:A:507:ASN:ND2	1:A:562:PHE:O	2.12	0.82
1:B:456:ILE:HB	1:B:460:GLU:HG3	1.60	0.81
1:B:126:VAL:HG23	1:B:127:MET:HG2	1.62	0.81
1:B:108:LEU:HD13	1:B:113:LEU:HD21	1.64	0.79
1:B:488:VAL:HG11	1:B:525:THR:HG21	1.66	0.77
1:B:502:VAL:HG13	1:B:513:ILE:HB	1.69	0.75
1:B:306:PRO:HG2	1:B:309:TRP:CD2	2.25	0.71
1:B:117:SER:O	2:B:601:HOH:O	2.08	0.71
1:A:297:THR:HG23	1:A:320:LYS:HB2	1.73	0.70
1:A:406:GLY:HA2	1:A:409:TYR:HD1	1.58	0.69
1:B:367:ILE:HG22	1:B:368:ARG:O	1.94	0.68
1:B:452:SER:N	2:B:605:HOH:O	2.27	0.66
1:B:531:ASP:OD1	1:B:533:HIS:ND1	2.28	0.66
1:B:536:GLY:HA3	1:B:543:ILE:HD11	1.78	0.66
1:B:73:ARG:HD3	1:B:86:LEU:HD22	1.79	0.65
1:B:174:THR:HG23	1:B:185:ARG:HB2	1.79	0.65
1:A:506:GLY:HA2	1:A:563:TYR:CE1	2.32	0.64
1:B:395:TYR:HB2	1:B:534:TYR:H	1.63	0.64
1:A:479:ASN:ND2	1:B:477:ALA:H	1.95	0.63
1:A:344:PRO:HD3	1:A:574:ALA:HB3	1.81	0.63
1:A:402:ASP:OD1	1:A:432:HIS:NE2	2.32	0.62
1:B:506:GLY:HA2	1:B:563:TYR:CD1	2.33	0.62
1:A:435:ILE:HG23	1:A:464:VAL:HG11	1.81	0.62
1:B:89:ASN:HB2	1:B:105:THR:HG23	1.82	0.62
1:B:176:LEU:HD13	1:B:216:MET:HE1	1.81	0.62
1:B:257:PRO:HG2	1:B:270:ARG:HD3	1.81	0.62
1:B:408:ALA:HB2	1:B:510:ALA:HB3	1.82	0.62
1:B:363:ASN:HB3	1:B:366:LEU:HD13	1.82	0.61
1:A:400:ILE:HG22	1:A:401:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASN:HB2	1:A:499:GLY:HA3	1.83	0.61
1:B:541:LYS:HA	1:B:544:THR:HG22	1.83	0.61
1:A:506:GLY:HA2	1:A:563:TYR:CD1	2.37	0.60
1:B:151:ARG:HH21	1:B:154:ARG:NH2	1.99	0.59
1:A:405:TRP:HA	1:A:455:TRP:HB3	1.85	0.58
1:A:455:TRP:HH2	1:B:456:ILE:HG22	1.68	0.58
1:B:73:ARG:NH2	1:B:77:GLU:OE2	2.35	0.58
1:B:504:ILE:HG13	1:B:565:MET:HG3	1.86	0.57
1:B:408:ALA:HB1	1:B:411:SER:HB3	1.86	0.57
1:A:507:ASN:CG	1:A:561:HIS:HB3	2.24	0.57
1:B:202:LYS:HG3	1:B:260:PHE:CE1	2.40	0.56
1:B:218:SER:OG	1:B:220:THR:HG22	2.05	0.56
1:B:389:PRO:HG2	1:B:421:LEU:HB3	1.86	0.56
1:A:420:ILE:HG22	1:A:425:THR:O	2.06	0.55
1:A:503:MET:HB3	1:A:566:VAL:HG13	1.88	0.55
1:A:407:CYS:SG	2:A:602:HOH:O	2.59	0.55
1:A:202:LYS:HG3	1:A:260:PHE:CE1	2.43	0.54
1:A:426:ASP:OD1	1:A:426:ASP:N	2.37	0.54
1:B:15:TRP:CD2	1:B:55:LYS:HG3	2.43	0.54
1:A:534:TYR:OH	1:A:537:SER:O	2.19	0.54
1:B:306:PRO:HG2	1:B:309:TRP:CG	2.43	0.53
1:A:456:ILE:HB	1:A:460:GLU:HG3	1.90	0.53
1:A:13:GLU:HB2	1:A:55:LYS:HE2	1.92	0.52
1:A:363:ASN:HB3	1:A:366:LEU:HD22	1.91	0.52
1:B:202:LYS:NZ	2:B:613:HOH:O	2.42	0.52
1:B:533:HIS:O	1:B:534:TYR:C	2.47	0.52
1:A:150:LEU:HD11	1:A:159:VAL:HG23	1.92	0.52
1:A:143:ARG:HG3	1:A:355:HIS:CE1	2.45	0.51
1:B:25:ASN:ND2	1:B:60:VAL:O	2.35	0.51
1:A:83:ASP:HB3	1:A:270:ARG:HD3	1.91	0.51
1:A:559:LYS:H	1:A:559:LYS:NZ	2.08	0.51
1:B:478:THR:HB	1:B:483:GLU:HB3	1.93	0.51
1:B:402:ASP:HA	1:B:405:TRP:NE1	2.26	0.51
1:A:412:PHE:CE1	1:A:465:LEU:HD13	2.46	0.51
1:B:30:ARG:NH2	1:B:114:GLU:OE2	2.42	0.51
1:A:177:ASN:HB3	1:A:182:LEU:HB2	1.93	0.51
1:A:378:GLN:N	1:A:379:PRO:HD3	2.26	0.51
1:A:425:THR:HG21	1:A:469:LEU:HD22	1.93	0.51
1:B:395:TYR:HB2	1:B:534:TYR:N	2.25	0.51
1:A:174:THR:OG1	1:A:185:ARG:HG3	2.11	0.50
1:B:506:GLY:HA2	1:B:563:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HD3	1:A:158:ASP:OD2	2.11	0.50
1:B:495:PHE:CE2	1:B:515:GLY:HA2	2.47	0.50
1:A:281:ASN:O	1:A:285:VAL:HG23	2.11	0.49
1:A:540:ILE:O	1:A:544:THR:HG22	2.11	0.49
1:A:161:SER:HA	1:A:164:GLU:HG3	1.95	0.49
1:B:286:THR:O	1:B:290:ILE:HG12	2.12	0.49
1:A:144:VAL:HG11	1:A:275:PHE:CE2	2.47	0.49
1:A:349:SER:OG	1:A:420:ILE:O	2.30	0.49
1:A:479:ASN:HD21	1:B:477:ALA:H	1.58	0.49
1:A:517:ASP:HB2	1:A:551:TRP:CZ3	2.48	0.49
1:A:297:THR:HG22	1:A:298:THR:O	2.12	0.48
1:B:329:TYR:CE2	1:B:333:LEU:HD11	2.49	0.48
1:B:70:GLU:O	1:B:74:GLN:HG2	2.14	0.48
1:A:18:ASP:HB2	1:A:133:VAL:HG23	1.96	0.48
1:B:386:VAL:HG23	1:B:499:GLY:O	2.14	0.48
1:A:504:ILE:HD12	1:A:565:MET:HG3	1.96	0.48
1:A:517:ASP:HB3	1:A:526:LYS:HB2	1.95	0.48
1:B:395:TYR:HE1	1:B:406:GLY:HA3	1.79	0.48
1:A:402:ASP:HA	1:A:405:TRP:NE1	2.30	0.47
1:A:485:VAL:C	1:A:487:ARG:H	2.17	0.47
1:B:457:GLY:O	1:B:460:GLU:HG2	2.14	0.47
1:A:360:ARG:NH2	2:A:612:HOH:O	2.48	0.47
1:A:389:PRO:HG2	1:A:421:LEU:HB3	1.97	0.47
1:A:507:ASN:OD1	1:B:459:THR:HB	2.14	0.47
1:B:171:PHE:HB2	1:B:268:TYR:OH	2.15	0.47
1:B:548:TRP:O	1:B:552:LYS:HE2	2.14	0.47
1:B:327:ARG:O	1:B:331:ILE:HG13	2.14	0.47
1:A:344:PRO:HG2	1:A:422:ASN:O	2.15	0.47
1:B:427:LYS:NZ	2:B:619:HOH:O	2.48	0.47
1:B:502:VAL:HG23	1:B:566:VAL:O	2.14	0.46
1:A:494:HIS:CE1	1:A:498:SER:HB2	2.51	0.46
1:B:536:GLY:HA3	1:B:543:ILE:CD1	2.45	0.46
1:B:282:THR:O	1:B:286:THR:HG23	2.15	0.46
1:B:368:ARG:HG2	1:B:369:GLU:H	1.80	0.46
1:B:129:ASN:ND2	2:B:621:HOH:O	2.49	0.46
1:B:526:LYS:HG2	1:B:553:PRO:HA	1.97	0.46
1:A:455:TRP:CH2	1:B:456:ILE:HG22	2.50	0.46
1:B:43:THR:HG21	2:B:684:HOH:O	2.16	0.46
1:A:416:TRP:CD1	1:A:429:VAL:HG12	2.50	0.46
1:A:552:LYS:HG2	1:A:556:PHE:CD1	2.51	0.46
1:B:416:TRP:CE2	1:B:430:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	2:A:610:HOH:O	2.46	0.45
1:A:452:SER:N	1:A:454:GLN:OE1	2.50	0.45
1:B:368:ARG:O	1:B:369:GLU:C	2.55	0.45
1:B:378:GLN:CD	1:B:378:GLN:O	2.55	0.45
1:A:479:ASN:HD22	1:B:477:ALA:HB3	1.82	0.45
1:A:294:ARG:HD3	1:A:325:GLU:CD	2.37	0.45
1:B:309:TRP:HA	2:B:609:HOH:O	2.17	0.45
1:B:394:HIS:O	1:B:410:ARG:NE	2.50	0.45
1:A:378:GLN:HB2	2:A:608:HOH:O	2.17	0.45
1:A:416:TRP:HD1	1:A:429:VAL:HG12	1.81	0.45
1:B:159:VAL:HG12	1:B:283:MET:HG2	1.98	0.44
1:B:514:LEU:HB2	1:B:528:LEU:HG	1.99	0.44
1:B:548:TRP:HB2	1:B:552:LYS:NZ	2.32	0.44
1:B:253:GLU:HG2	1:B:301:SER:HB3	1.98	0.44
1:A:150:LEU:HB3	1:A:155:GLU:HA	2.00	0.44
1:A:429:VAL:HA	1:A:430:PRO:HD3	1.81	0.44
1:B:396:MET:HB3	1:B:401:ASP:OD1	2.17	0.44
1:A:54:ARG:HD2	2:A:703:HOH:O	2.18	0.44
1:B:395:TYR:HB2	1:B:534:TYR:HB2	1.99	0.44
1:B:395:TYR:CE1	1:B:406:GLY:HA3	2.53	0.44
1:B:540:ILE:O	1:B:540:ILE:HG12	2.16	0.44
1:A:531:ASP:HA	1:A:532:PRO:HD3	1.80	0.44
1:B:398:ASP:N	1:B:398:ASP:OD1	2.51	0.44
1:B:145:GLY:HA2	1:B:250:THR:O	2.18	0.43
1:B:570:PRO:HA	1:B:571:PRO:HD3	1.88	0.43
1:A:490:GLU:H	1:A:490:GLU:HG2	1.68	0.43
1:B:187:GLN:HB2	1:B:191:ALA:HB3	2.01	0.43
1:B:368:ARG:NH1	2:B:625:HOH:O	2.51	0.43
1:B:378:GLN:HA	1:B:379:PRO:HD2	1.87	0.43
1:A:90:LEU:HD13	1:A:108:LEU:HD12	2.00	0.43
1:A:409:TYR:O	1:A:412:PHE:HB3	2.18	0.43
1:B:488:VAL:HB	1:B:516:VAL:HG21	2.00	0.43
1:A:476:ILE:HG23	1:A:487:ARG:NH1	2.34	0.43
1:A:539:ASP:HB3	1:A:542:THR:OG1	2.19	0.43
1:A:487:ARG:HG3	1:A:490:GLU:OE2	2.19	0.42
1:B:62:PHE:CE2	1:B:90:LEU:HD11	2.54	0.42
1:B:306:PRO:O	1:B:309:TRP:HB2	2.18	0.42
1:A:150:LEU:HD21	1:A:159:VAL:HG23	2.01	0.42
1:A:394:HIS:O	1:A:410:ARG:NE	2.53	0.42
1:A:456:ILE:HB	1:A:460:GLU:CG	2.48	0.42
1:A:322:THR:HG23	1:A:325:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLU:OE1	1:B:190:GLU:N	2.52	0.42
1:B:456:ILE:HB	1:B:460:GLU:CG	2.42	0.42
1:B:519:ASN:OD1	1:B:522:THR:HB	2.20	0.42
1:A:454:GLN:NE2	1:A:454:GLN:H	2.18	0.42
1:A:73:ARG:NH1	1:A:77:GLU:OE2	2.53	0.42
1:B:151:ARG:HH21	1:B:154:ARG:CZ	2.33	0.42
1:B:493:ARG:NH1	1:B:496:GLU:OE2	2.53	0.42
1:A:507:ASN:ND2	1:A:561:HIS:HB3	2.34	0.42
1:B:395:TYR:O	1:B:396:MET:HG2	2.20	0.42
1:B:539:ASP:OD1	1:B:542:THR:HG23	2.19	0.42
1:B:300:THR:HG23	1:B:319:THR:OG1	2.20	0.42
1:B:121:PHE:CE1	1:B:125:ASN:ND2	2.86	0.42
1:A:476:ILE:HG23	1:A:487:ARG:HH11	1.85	0.41
1:A:505:GLY:N	1:A:564:ASN:O	2.35	0.41
1:A:478:THR:O	1:A:562:PHE:HB2	2.20	0.41
1:B:344:PRO:HG2	1:B:422:ASN:O	2.19	0.41
1:A:409:TYR:HD2	1:A:435:ILE:HD12	1.85	0.41
1:B:121:PHE:HE1	1:B:125:ASN:ND2	2.19	0.41
1:B:339:LEU:HD13	1:B:345:VAL:HG21	2.03	0.41
1:B:377:TYR:HB3	1:B:378:GLN:H	1.68	0.41
1:B:218:SER:CB	1:B:220:THR:HG22	2.50	0.41
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.93	0.41
1:B:407:CYS:HA	1:B:408:ALA:HA	1.72	0.41
1:B:514:LEU:HD11	1:B:530:LEU:HB2	2.03	0.41
1:A:480:SER:HA	1:A:561:HIS:O	2.21	0.41
1:B:193:GLN:O	1:B:196:TYR:HB2	2.21	0.40
1:A:343:LYS:HB2	1:A:344:PRO:HD2	2.03	0.40
1:A:565:MET:HE3	1:A:565:MET:HB2	1.88	0.40
1:B:531:ASP:HA	1:B:532:PRO:HD2	1.95	0.40
1:A:459:THR:HB	1:B:562:PHE:HE1	1.87	0.40
1:B:111:ARG:HG2	1:B:115:ASN:ND2	2.36	0.40
1:B:405:TRP:CZ3	1:B:453:ARG:HA	2.57	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	509/564 (90%)	472 (93%)	37 (7%)	0	100	100
1	B	512/564 (91%)	459 (90%)	53 (10%)	0	100	100
All	All	1021/1128 (90%)	931 (91%)	90 (9%)	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	449/494 (91%)	420 (94%)	29 (6%)	17	44
1	B	453/494 (92%)	423 (93%)	30 (7%)	16	44
All	All	902/988 (91%)	843 (94%)	59 (6%)	17	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLU
1	A	86	LEU
1	A	113	LEU
1	A	119	SER
1	A	124	MET
1	A	164	GLU
1	A	168	MET
1	A	246	THR
1	A	251	ILE
1	A	283	MET
1	A	301	SER
1	A	348	LEU
1	A	349	SER
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	377	TYR
1	A	378	GLN
1	A	402	ASP
1	A	420	ILE
1	A	426	ASP
1	A	429	VAL
1	A	452	SER
1	A	459	THR
1	A	470	LYS
1	A	487	ARG
1	A	488	VAL
1	A	534	TYR
1	A	537	SER
1	A	560	ASP
1	B	42	THR
1	B	60	VAL
1	B	81	SER
1	B	97	GLN
1	B	117	SER
1	B	146	TYR
1	B	157	GLU
1	B	176	LEU
1	B	205	VAL
1	B	210	VAL
1	B	219	LEU
1	B	268	TYR
1	B	301	SER
1	B	303	THR
1	B	341	SER
1	B	364	LYS
1	B	378	GLN
1	B	398	ASP
1	B	421	LEU
1	B	454	GLN
1	B	455	TRP
1	B	459	THR
1	B	509	LEU
1	B	512	THR
1	B	518	PHE
1	B	540	ILE
1	B	548	TRP

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Mol	Chain	Res	Type
1	B	561	HIS
1	B	562	PHE
1	B	575	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	564	ASN
1	B	564	ASN

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	517/564 (91%)	-0.12	11 (2%)	63	54	8, 40, 87, 132	0
1	B	520/564 (92%)	-0.08	5 (0%)	82	77	11, 42, 96, 128	0
All	All	1037/1128 (91%)	-0.10	16 (1%)	73	68	8, 41, 90, 132	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	TRP	5.5
1	A	535	THR	5.5
1	A	159	VAL	3.2
1	B	489	ARG	2.8
1	A	537	SER	2.8
1	B	521	THR	2.8
1	A	507	ASN	2.8
1	A	245	PHE	2.8
1	B	546	LYS	2.7
1	A	152	ALA	2.5
1	A	400	ILE	2.5
1	B	454	GLN	2.5
1	A	247	ARG	2.3
1	A	542	THR	2.3
1	A	470	LYS	2.2
1	A	534	TYR	2.2

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.