Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 04:10 PM EST

PDB ID	:	3OQC
Title	:	Ubiquitin-fold modifier 1 Specific Protease, UfSP2
Authors	:	Ha, B.H.; Chung, C.H.; Kim, E.E.
Deposited on	:	2010-09-02
Resolution	:	2.60 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 ⓘ 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 ⓘ) were used in the production of this report:

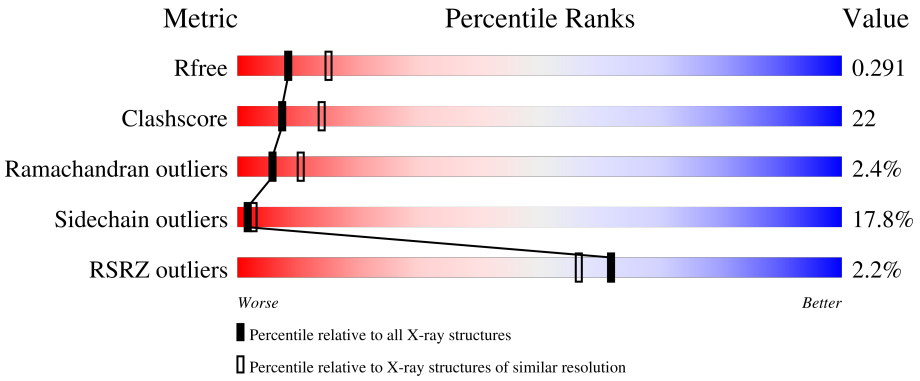
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	481	2% 48% 29% 9% 14%
1	B	481	2% 50% 28% 7% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6716 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3328	2131	573	606	18			
1	B	411	Total	C	N	O	S	0	0	0
			3281	2101	561	601	18			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q99K23
A	-18	GLY	-	expression tag	UNP Q99K23
A	-17	SER	-	expression tag	UNP Q99K23
A	-16	SER	-	expression tag	UNP Q99K23
A	-15	HIS	-	expression tag	UNP Q99K23
A	-14	HIS	-	expression tag	UNP Q99K23
A	-13	HIS	-	expression tag	UNP Q99K23
A	-12	HIS	-	expression tag	UNP Q99K23
A	-11	HIS	-	expression tag	UNP Q99K23
A	-10	HIS	-	expression tag	UNP Q99K23
A	-9	SER	-	expression tag	UNP Q99K23
A	-8	SER	-	expression tag	UNP Q99K23
A	-7	GLY	-	expression tag	UNP Q99K23
A	-6	LEU	-	expression tag	UNP Q99K23
A	-5	VAL	-	expression tag	UNP Q99K23
A	-4	PRO	-	expression tag	UNP Q99K23
A	-3	ARG	-	expression tag	UNP Q99K23
A	-2	GLY	-	expression tag	UNP Q99K23
A	-1	SER	-	expression tag	UNP Q99K23
A	0	HIS	-	expression tag	UNP Q99K23
A	94	ARG	LYS	engineered mutation	UNP Q99K23
A	128	ALA	ARG	engineered mutation	UNP Q99K23
A	294	SER	CYS	engineered mutation	UNP Q99K23
B	-19	MET	-	expression tag	UNP Q99K23
B	-18	GLY	-	expression tag	UNP Q99K23

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q99K23
B	-16	SER	-	expression tag	UNP Q99K23
B	-15	HIS	-	expression tag	UNP Q99K23
B	-14	HIS	-	expression tag	UNP Q99K23
B	-13	HIS	-	expression tag	UNP Q99K23
B	-12	HIS	-	expression tag	UNP Q99K23
B	-11	HIS	-	expression tag	UNP Q99K23
B	-10	HIS	-	expression tag	UNP Q99K23
B	-9	SER	-	expression tag	UNP Q99K23
B	-8	SER	-	expression tag	UNP Q99K23
B	-7	GLY	-	expression tag	UNP Q99K23
B	-6	LEU	-	expression tag	UNP Q99K23
B	-5	VAL	-	expression tag	UNP Q99K23
B	-4	PRO	-	expression tag	UNP Q99K23
B	-3	ARG	-	expression tag	UNP Q99K23
B	-2	GLY	-	expression tag	UNP Q99K23
B	-1	SER	-	expression tag	UNP Q99K23
B	0	HIS	-	expression tag	UNP Q99K23
B	94	ARG	LYS	engineered mutation	UNP Q99K23
B	128	ALA	ARG	engineered mutation	UNP Q99K23
B	294	SER	CYS	engineered mutation	UNP Q99K23

- Molecule 2 is water.

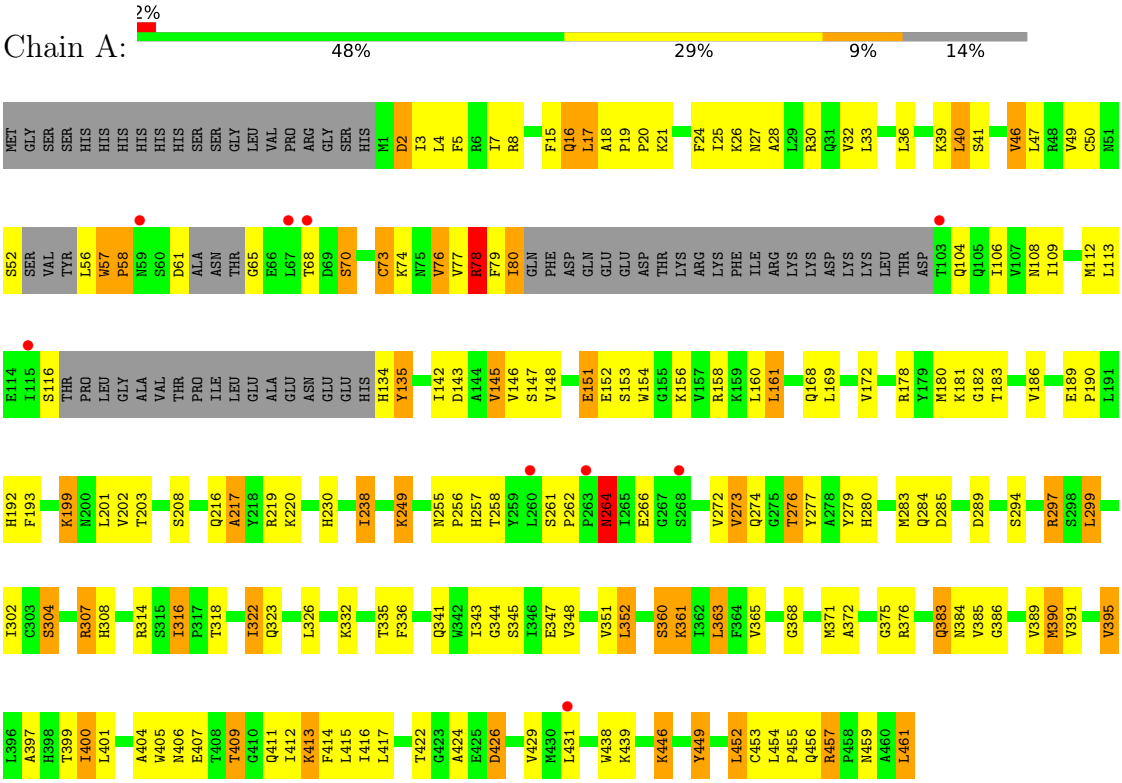
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	53	Total O 53 53	0	0
2	B	54	Total O 54 54	0	0

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.

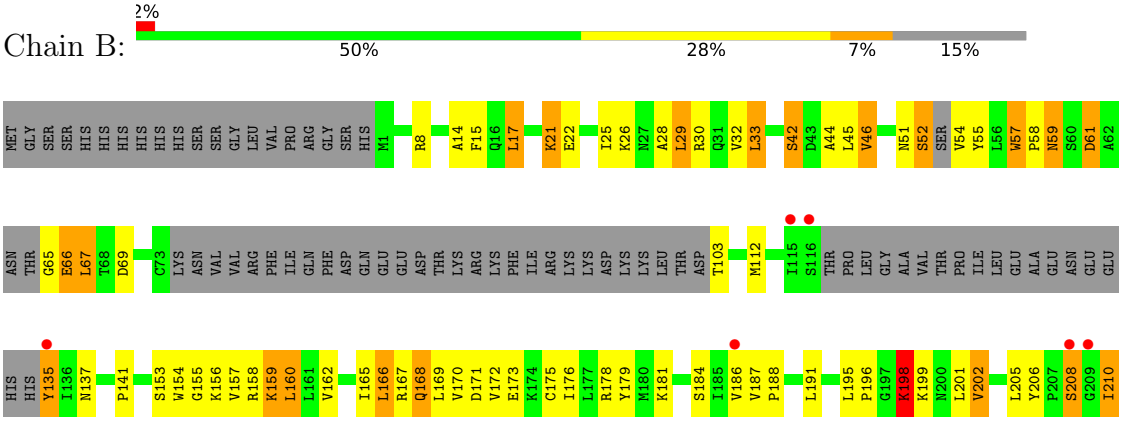
• Molecule 1: Ufm1-specific protease 2

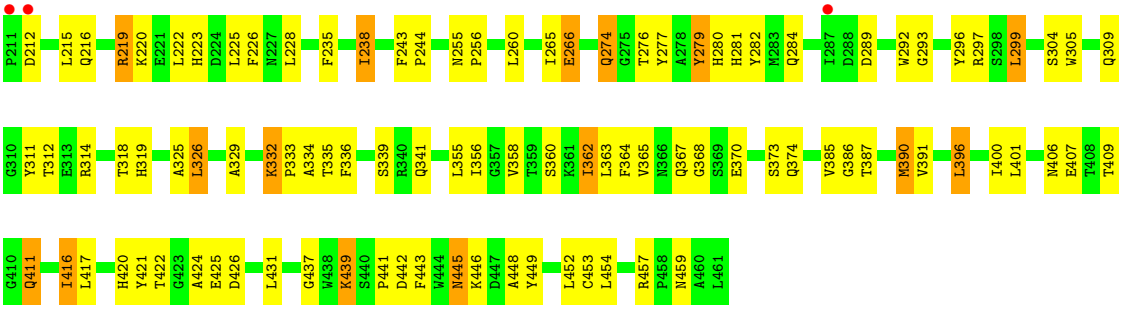
Chain A:



• Molecule 1: Ufm1-specific protease 2

Chain B:




P211 D212 L215 Q216 R219 K220 E221 L222 H223 D224 L225 F226 N227 L228 F235 I238 F243 P244 N255 P256 L260 I265 E266 Q274 G275 T276 Y277 A278 Y279 H280 H281 Y282 M283 Q284 I287 D288 D289 W292 G293 Y296 R297 S298 L299 S304 W305 Q309
G310 Y311 T312 E313 R314 T318 H319 A325 L326 A329 K332 P333 A334 T335 F336 S339 R340 Q341 L355 I356 G357 V358 T359 S360 K361 I362 L363 F364 V365 N366 Q367 G368 S369 E370 S373 Q374 V385 G386 T387 M390 V391 L396 I400 L401 N406 E407 T408 T409
G410 Q411 I416 L417 H420 Y421 T422 G423 A424 E425 D426 L431 G437 W438 K439 S440 P441 D442 F443 W444 N445 K446 D447 A448 Y449 L452 C453 L454 R457 P458 N459 A460 L461

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.53Å 56.04Å 143.27Å 90.00° 128.01° 90.00°	Depositor
Resolution (Å)	46.10 – 2.60 46.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.10-2.60) 98.4 (46.10-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.238 , 0.298 0.233 , 0.291	Depositor DCC
R_{free} test set	1776 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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

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	0.76	1/3409 (0.0%)	0.85	1/4627 (0.0%)
1	B	0.71	0/3361	0.84	4/4564 (0.1%)
All	All	0.74	1/6770 (0.0%)	0.84	5/9191 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLY	N-CA	6.91	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	B	396	LEU	CA-CB-CG	5.44	127.80	115.30
1	B	8	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	201	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	457	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	PRO	Peptide
1	A	57	TRP	Peptide
1	B	57	TRP	Peptide

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	3328	0	3297	167	1
1	B	3281	0	3243	126	0
2	A	53	0	0	15	0
2	B	54	0	0	10	1
All	All	6716	0	6540	293	1

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 22.

All (293) 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:65:GLY:HA2	1:B:158:ARG:HH12	0.99	1.09
1:B:409:THR:HG21	2:B:494:HOH:O	1.50	1.08
1:B:260:LEU:HD11	1:B:437:GLY:HA2	1.37	1.07
1:A:216:GLN:HB2	2:A:476:HOH:O	1.58	1.03
1:B:362:ILE:HD11	1:B:364:PHE:CZ	1.94	1.02
1:A:49:VAL:HB	1:A:58:PRO:CG	1.90	1.00
1:A:383:GLN:HE21	1:A:383:GLN:HA	1.22	1.00
1:B:219:ARG:HH11	1:B:219:ARG:HB2	1.26	0.98
1:B:65:GLY:HA2	1:B:158:ARG:NH1	1.78	0.97
1:B:362:ILE:HD11	1:B:364:PHE:CE1	2.04	0.92
1:A:426:ASP:HB3	2:A:487:HOH:O	1.70	0.92
1:A:17:LEU:HD13	1:A:25:ILE:HG23	1.49	0.91
1:A:322:ILE:HD12	1:A:351:VAL:HG21	1.55	0.89
1:A:49:VAL:HB	1:A:58:PRO:HG2	1.55	0.88
1:B:219:ARG:HA	1:B:222:LEU:HD12	1.55	0.88
1:A:406:ASN:HB3	1:A:409:THR:HG22	1.54	0.88
1:B:219:ARG:HH11	1:B:219:ARG:CB	1.88	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:CD2	1:A:352:LEU:HD13	2.07	0.85
1:A:52:SER:HA	1:A:79:PHE:CD2	2.11	0.85
1:B:219:ARG:HB2	1:B:219:ARG:NH1	1.93	0.83
1:A:446:LYS:H	1:A:446:LYS:HD3	1.44	0.83
1:B:198:LYS:HE3	1:B:198:LYS:O	1.80	0.82
1:A:449:TYR:HB2	2:A:462:HOH:O	1.79	0.81
1:B:289:ASP:HA	1:B:292:TRP:CE2	2.17	0.80
1:A:383:GLN:HA	1:A:383:GLN:NE2	1.98	0.79
1:B:363:LEU:HD12	2:B:516:HOH:O	1.82	0.79
1:B:452:LEU:HD22	2:B:516:HOH:O	1.82	0.79
1:A:158:ARG:HD3	2:A:488:HOH:O	1.83	0.78
1:A:19:PRO:HB2	1:A:20:PRO:HD3	1.65	0.77
1:A:283:MET:HG3	1:A:422:THR:HG23	1.66	0.77
1:A:15:PHE:HB3	1:A:32:VAL:HG21	1.65	0.77
1:B:370:GLU:O	1:B:373:SER:HB2	1.84	0.77
1:B:289:ASP:OD1	1:B:297:ARG:HD3	1.85	0.76
1:A:219:ARG:NH1	1:A:461:LEU:OXT	2.18	0.75
1:A:52:SER:HA	1:A:79:PHE:HD2	1.51	0.74
1:A:299:LEU:HD21	1:A:352:LEU:HD13	1.69	0.74
1:A:406:ASN:HB3	1:A:409:THR:CG2	2.18	0.72
1:A:16:GLN:HG3	1:A:135:TYR:HD1	1.54	0.72
1:B:289:ASP:HA	1:B:292:TRP:NE1	2.04	0.72
1:A:78:ARG:HH11	1:A:78:ARG:HB3	1.54	0.72
1:A:429:VAL:HG23	2:A:487:HOH:O	1.90	0.70
1:A:49:VAL:CB	1:A:58:PRO:HG2	2.21	0.70
1:A:391:VAL:HG12	1:A:452:LEU:HD22	1.74	0.70
1:B:198:LYS:HA	2:B:480:HOH:O	1.92	0.70
1:B:416:ILE:HD11	1:B:439:LYS:HD3	1.73	0.70
1:A:255:ASN:O	1:A:258:THR:HG22	1.93	0.69
1:A:409:THR:HG23	1:A:411:GLN:H	1.59	0.68
1:A:189:GLU:OE2	1:A:208:SER:HB2	1.94	0.68
1:B:362:ILE:CD1	1:B:364:PHE:CE1	2.77	0.68
1:A:274:GLN:HG3	1:A:457:ARG:HH21	1.60	0.67
1:B:238:ILE:O	1:B:238:ILE:HG13	1.92	0.67
1:A:322:ILE:HG13	1:A:323:GLN:N	2.09	0.67
1:B:42:SER:HB2	1:B:44:ALA:H	1.61	0.66
1:A:16:GLN:CG	1:A:135:TYR:HD1	2.07	0.66
1:A:255:ASN:OD1	1:A:276:THR:HB	1.96	0.66
1:A:299:LEU:HG	1:A:348:VAL:HG13	1.76	0.66
1:A:70:SER:HB3	1:A:153:SER:HB2	1.77	0.65
1:A:16:GLN:HG3	1:A:135:TYR:CD1	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HB	1:A:58:PRO:HG3	1.78	0.64
1:A:216:GLN:CB	2:A:476:HOH:O	2.27	0.64
1:B:65:GLY:CA	1:B:158:ARG:HH12	1.93	0.64
1:B:407:GLU:HB3	2:B:463:HOH:O	1.99	0.63
1:A:49:VAL:CG2	1:A:58:PRO:HG2	2.28	0.63
1:B:374:GLN:HA	1:B:374:GLN:NE2	2.13	0.62
1:B:168:GLN:O	1:B:172:VAL:HG23	1.99	0.62
1:B:202:VAL:HG21	1:B:226:PHE:CZ	2.35	0.62
1:B:216:GLN:HA	1:B:219:ARG:HH12	1.65	0.62
1:A:219:ARG:NH2	2:A:476:HOH:O	2.32	0.62
1:B:282:TYR:HB2	1:B:421:TYR:O	2.00	0.61
1:A:372:ALA:HA	1:A:412:ILE:HG21	1.82	0.61
1:A:199:LYS:HE3	1:A:199:LYS:O	2.00	0.61
1:B:390:MET:HG3	1:B:453:CYS:HB3	1.83	0.60
1:B:282:TYR:CD1	1:B:420:HIS:HA	2.36	0.60
1:B:391:VAL:O	1:B:391:VAL:HG23	2.00	0.60
1:A:8:ARG:HH21	1:A:108:ASN:ND2	1.99	0.60
1:A:274:GLN:HG2	1:A:386:GLY:HA3	1.83	0.60
1:A:376:ARG:NH2	1:A:407:GLU:OE1	2.34	0.60
1:A:255:ASN:O	1:A:258:THR:CG2	2.51	0.59
1:B:265:ILE:HG22	1:B:266:GLU:O	2.03	0.59
1:B:274:GLN:HG2	1:B:386:GLY:HA3	1.85	0.59
1:A:449:TYR:CD1	1:A:449:TYR:C	2.76	0.59
1:A:257:HIS:HB2	1:A:415:LEU:HD21	1.86	0.58
1:A:143:ASP:HB3	1:A:190:PRO:HG2	1.86	0.58
1:A:220:LYS:HG2	1:A:461:LEU:HD11	1.85	0.58
1:A:17:LEU:HD13	1:A:25:ILE:CG2	2.28	0.57
1:B:59:ASN:HB2	2:B:503:HOH:O	2.04	0.57
1:B:391:VAL:HG12	1:B:452:LEU:HG	1.86	0.57
1:B:362:ILE:HA	1:B:452:LEU:O	2.04	0.57
1:A:49:VAL:O	1:A:52:SER:OG	2.18	0.56
1:B:305:TRP:O	1:B:309:GLN:HG2	2.04	0.56
1:A:25:ILE:HA	1:A:28:ALA:HB3	1.86	0.56
1:B:45:LEU:O	1:B:58:PRO:HD3	2.04	0.56
1:B:61:ASP:N	1:B:61:ASP:OD2	2.38	0.56
1:B:219:ARG:HD3	1:B:235:PHE:C	2.25	0.56
1:B:452:LEU:N	1:B:452:LEU:HD12	2.20	0.56
1:B:175:CYS:SG	1:B:188:PRO:HG3	2.46	0.56
1:A:274:GLN:HG3	1:A:457:ARG:NH2	2.20	0.56
1:B:336:PHE:O	1:B:339:SER:CB	2.53	0.56
1:B:284:GLN:HB2	1:B:297:ARG:NH2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:CB	1:A:32:VAL:HG21	2.33	0.56
1:A:400:ILE:HD12	1:A:415:LEU:O	2.06	0.56
1:A:304:SER:HA	1:A:307:ARG:HG2	1.88	0.56
1:B:162:VAL:O	1:B:166:LEU:HD22	2.06	0.56
1:B:176:ILE:HA	2:B:496:HOH:O	2.05	0.56
1:A:4:LEU:HD23	1:A:106:ILE:HD13	1.89	0.55
1:A:375:GLY:HA3	1:A:412:ILE:HD12	1.89	0.55
1:B:364:PHE:HD2	1:B:449:TYR:HH	1.54	0.55
1:A:383:GLN:HE21	1:A:383:GLN:CA	2.05	0.55
1:A:25:ILE:HD12	1:A:26:LYS:H	1.72	0.55
1:A:46:VAL:HG22	1:A:112:MET:HE3	1.89	0.54
1:A:216:GLN:CA	2:A:476:HOH:O	2.51	0.54
1:B:51:ASN:O	1:B:52:SER:HB2	2.08	0.54
1:A:168:GLN:O	1:A:172:VAL:HG23	2.07	0.54
1:B:409:THR:HG23	1:B:411:GLN:H	1.72	0.54
1:B:336:PHE:HE1	1:B:341:GLN:HB2	1.73	0.54
1:A:401:LEU:HD11	1:A:417:LEU:HB2	1.90	0.54
1:B:256:PRO:HD2	1:B:277:TYR:OH	2.07	0.54
1:B:368:GLY:HA3	1:B:445:ASN:O	2.08	0.54
1:A:376:ARG:HH21	1:A:405:TRP:HZ3	1.55	0.53
1:B:216:GLN:HA	1:B:219:ARG:NH1	2.23	0.53
1:B:385:VAL:HG12	1:B:387:THR:HG23	1.89	0.53
1:B:14:ALA:CB	1:B:137:ASN:OD1	2.56	0.53
1:B:17:LEU:HD12	1:B:21:LYS:HB2	1.90	0.53
1:A:79:PHE:CB	2:A:477:HOH:O	2.56	0.53
1:B:66:GLU:HB3	1:B:154:TRP:HD1	1.72	0.53
1:A:401:LEU:O	1:A:415:LEU:HD23	2.09	0.53
1:A:52:SER:CA	1:A:79:PHE:HD2	2.21	0.53
1:B:181:LYS:HB3	1:B:184:SER:OG	2.08	0.53
1:B:336:PHE:O	1:B:339:SER:HB3	2.09	0.53
1:A:52:SER:CA	1:A:79:PHE:CD2	2.86	0.52
1:B:279:TYR:CE2	1:B:281:HIS:HB3	2.44	0.52
1:A:49:VAL:HB	1:A:58:PRO:CD	2.40	0.52
1:B:195:LEU:HD22	1:B:228:LEU:HD11	1.92	0.52
1:B:401:LEU:HD11	1:B:417:LEU:HB2	1.92	0.52
1:A:280:HIS:NE2	1:A:316:ILE:HD12	2.24	0.52
1:A:360:SER:HB3	1:A:455:PRO:HA	1.92	0.52
1:B:67:LEU:HD22	1:B:67:LEU:H	1.75	0.52
1:A:348:VAL:HG11	1:A:390:MET:HG2	1.92	0.52
1:B:280:HIS:HA	1:B:284:GLN:HE22	1.75	0.52
1:B:153:SER:O	1:B:157:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:HB3	1:B:205:LEU:HD12	1.92	0.51
1:B:445:ASN:C	1:B:445:ASN:HD22	2.12	0.51
1:A:79:PHE:HB2	2:A:477:HOH:O	2.11	0.51
1:B:445:ASN:OD1	1:B:448:ALA:HB2	2.11	0.51
1:B:191:LEU:HD12	1:B:206:TYR:HB2	1.93	0.51
1:A:68:THR:OG1	1:A:158:ARG:NH2	2.44	0.51
1:B:445:ASN:ND2	1:B:446:LYS:O	2.44	0.51
1:A:272:VAL:HG23	1:A:401:LEU:O	2.10	0.51
1:B:299:LEU:HD23	1:B:299:LEU:O	2.11	0.51
1:A:216:GLN:N	2:A:476:HOH:O	2.44	0.50
1:B:14:ALA:HB2	1:B:137:ASN:OD1	2.11	0.50
1:A:256:PRO:HD2	1:A:277:TYR:CZ	2.47	0.50
1:B:166:LEU:O	1:B:167:ARG:C	2.50	0.50
1:B:441:PRO:C	1:B:443:PHE:H	2.14	0.50
1:A:68:THR:HG23	1:A:158:ARG:HE	1.77	0.50
1:B:356:ILE:HG13	1:B:358:VAL:HG23	1.94	0.50
1:A:414:PHE:O	1:A:438:TRP:HA	2.11	0.49
1:A:409:THR:CG2	1:A:411:GLN:HB2	2.42	0.49
1:A:409:THR:CG2	1:A:411:GLN:H	2.23	0.49
1:B:416:ILE:HD11	1:B:439:LYS:HB2	1.94	0.49
1:B:173:GLU:OE2	2:B:473:HOH:O	2.20	0.49
1:A:17:LEU:HD12	1:A:21:LYS:HD2	1.93	0.49
1:A:336:PHE:CE1	1:A:341:GLN:HB2	2.47	0.49
1:A:289:ASP:CG	1:A:297:ARG:NH1	2.66	0.49
1:B:289:ASP:HA	1:B:292:TRP:CZ2	2.48	0.49
1:A:8:ARG:HA	1:A:142:ILE:O	2.12	0.49
1:A:18:ALA:HB3	1:A:24:PHE:CE1	2.47	0.48
1:A:322:ILE:CD1	1:A:351:VAL:HG21	2.36	0.48
1:B:374:GLN:NE2	1:B:374:GLN:CA	2.75	0.48
1:A:25:ILE:HD12	1:A:26:LYS:N	2.28	0.48
1:B:279:TYR:CD1	1:B:417:LEU:HD11	2.47	0.48
1:B:325:ALA:HB2	1:B:355:LEU:HD21	1.96	0.48
1:B:336:PHE:CE1	1:B:341:GLN:HB2	2.48	0.48
1:B:26:LYS:O	1:B:30:ARG:HG3	2.12	0.48
1:A:151:GLU:O	1:A:152:GLU:C	2.52	0.48
1:A:406:ASN:ND2	1:A:409:THR:HB	2.29	0.48
1:B:219:ARG:HD3	1:B:235:PHE:O	2.13	0.48
1:A:146:VAL:HG11	1:A:161:LEU:HD12	1.95	0.48
1:A:272:VAL:HG22	1:A:273:VAL:H	1.79	0.47
1:A:73:CYS:HB2	1:A:152:GLU:O	2.13	0.47
1:B:277:TYR:CD2	1:B:277:TYR:C	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG21	1:A:352:LEU:HD21	1.95	0.47
1:B:141:PRO:HD3	1:B:187:VAL:HG11	1.96	0.47
1:B:65:GLY:CA	1:B:158:ARG:NH1	2.64	0.47
1:A:363:LEU:HB3	1:A:452:LEU:HB2	1.96	0.47
1:B:178:ARG:HD3	1:B:179:TYR:CZ	2.49	0.47
1:B:141:PRO:HD3	1:B:187:VAL:CG1	2.44	0.47
1:A:453:CYS:C	1:A:454:LEU:HD12	2.35	0.47
1:B:255:ASN:N	1:B:256:PRO:HD3	2.29	0.47
1:A:376:ARG:HB2	1:A:405:TRP:CH2	2.49	0.47
1:A:73:CYS:O	1:A:76:VAL:HG23	2.15	0.47
1:A:318:THR:O	1:A:322:ILE:HG23	2.15	0.47
1:B:206:TYR:CE1	1:B:215:LEU:HD13	2.50	0.47
1:A:52:SER:C	1:A:79:PHE:CE2	2.89	0.46
1:A:76:VAL:O	1:A:78:ARG:N	2.48	0.46
1:A:219:ARG:NH1	1:A:461:LEU:C	2.68	0.46
1:B:336:PHE:O	1:B:339:SER:HB2	2.15	0.46
1:A:284:GLN:HB2	1:A:297:ARG:NH2	2.31	0.46
1:B:406:ASN:CG	1:B:409:THR:HG22	2.36	0.46
1:A:15:PHE:CG	1:A:32:VAL:HG21	2.50	0.46
1:A:389:VAL:HB	1:A:400:ILE:HG23	1.98	0.46
1:A:189:GLU:HB2	2:A:471:HOH:O	2.15	0.46
1:A:216:GLN:O	1:A:217:ALA:C	2.54	0.46
1:A:391:VAL:HG12	1:A:452:LEU:CD2	2.45	0.46
1:B:29:LEU:O	1:B:33:LEU:HB2	2.16	0.46
1:A:18:ALA:HB3	1:A:24:PHE:CD1	2.52	0.45
1:A:289:ASP:OD2	1:A:297:ARG:NH1	2.49	0.45
1:A:56:LEU:HG	2:A:489:HOH:O	2.16	0.45
1:A:449:TYR:C	1:A:449:TYR:HD1	2.19	0.45
1:A:3:ILE:HG22	1:A:148:VAL:O	2.17	0.45
1:B:67:LEU:H	1:B:67:LEU:CD2	2.29	0.45
1:B:220:LYS:O	1:B:223:HIS:HB2	2.17	0.45
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.82	0.45
1:B:28:ALA:O	1:B:32:VAL:HG23	2.17	0.45
1:B:424:ALA:O	1:B:426:ASP:N	2.41	0.45
1:A:3:ILE:HG21	1:A:73:CYS:SG	2.56	0.45
1:A:449:TYR:CD1	1:A:449:TYR:O	2.69	0.45
1:B:14:ALA:HB2	1:B:137:ASN:HA	1.99	0.45
1:B:25:ILE:O	1:B:29:LEU:HB2	2.17	0.45
1:A:4:LEU:HD23	1:A:106:ILE:CD1	2.46	0.44
1:A:238:ILE:HG23	1:A:308:HIS:O	2.18	0.44
1:A:52:SER:C	1:A:79:PHE:CD2	2.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:HIS:CE1	1:A:316:ILE:HD12	2.52	0.44
1:B:159:LYS:O	1:B:162:VAL:HG12	2.17	0.44
1:B:219:ARG:O	1:B:222:LEU:HB2	2.18	0.44
1:A:390:MET:HG3	1:A:453:CYS:HB3	1.98	0.44
1:B:238:ILE:O	1:B:238:ILE:CG1	2.62	0.44
1:B:445:ASN:C	1:B:445:ASN:ND2	2.71	0.44
1:B:135:TYR:N	1:B:135:TYR:CD1	2.84	0.44
1:B:326:LEU:O	1:B:329:ALA:N	2.50	0.44
1:A:389:VAL:HG13	1:A:453:CYS:O	2.18	0.43
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.82	0.43
1:B:157:VAL:O	1:B:160:LEU:N	2.52	0.43
1:B:33:LEU:HD13	1:B:33:LEU:HA	1.78	0.43
1:A:156:LYS:O	1:A:160:LEU:HG	2.19	0.43
1:B:311:TYR:OH	1:B:457:ARG:HD3	2.19	0.43
1:A:5:PHE:HD1	1:A:109:ILE:HD11	1.84	0.43
1:A:390:MET:CE	1:A:397:ALA:HB1	2.48	0.43
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.82	0.43
1:A:46:VAL:HG22	1:A:112:MET:CE	2.49	0.43
1:A:401:LEU:HB2	1:A:415:LEU:HD23	2.01	0.42
1:A:361:LYS:HE3	1:A:361:LYS:HB3	1.79	0.42
1:A:249:LYS:CD	1:A:249:LYS:H	2.31	0.42
1:A:289:ASP:CG	1:A:297:ARG:HH11	2.23	0.42
1:B:210:ILE:O	1:B:215:LEU:HD11	2.19	0.42
1:B:274:GLN:HE21	1:B:274:GLN:HB3	1.73	0.42
1:A:49:VAL:H	1:A:58:PRO:HD2	1.83	0.42
1:A:456:GLN:NE2	2:A:490:HOH:O	2.06	0.42
1:B:284:GLN:CB	1:B:297:ARG:NH2	2.83	0.42
1:A:375:GLY:CA	1:A:412:ILE:HD12	2.49	0.42
1:B:155:GLY:O	1:B:158:ARG:HG2	2.19	0.42
1:A:49:VAL:O	1:A:49:VAL:HG12	2.20	0.42
1:A:255:ASN:HD21	1:A:276:THR:HA	1.84	0.42
1:A:375:GLY:CA	1:A:412:ILE:CD1	2.98	0.42
1:B:54:VAL:CG1	1:B:55:TYR:N	2.82	0.42
1:B:293:GLY:HA2	1:B:296:TYR:CD2	2.55	0.42
1:A:79:PHE:CD1	1:A:80:ILE:N	2.88	0.42
1:B:445:ASN:HD22	1:B:446:LYS:N	2.17	0.42
1:B:454:LEU:N	1:B:454:LEU:HD12	2.34	0.42
1:A:368:GLY:HA3	1:A:446:LYS:HA	2.01	0.41
1:A:5:PHE:HB2	1:A:146:VAL:HG13	2.00	0.41
1:A:277:TYR:CD2	1:A:277:TYR:C	2.93	0.41
1:B:186:VAL:O	1:B:188:PRO:HD3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:HB3	1:A:32:VAL:CG2	2.44	0.41
1:A:21:LYS:O	1:A:25:ILE:HG13	2.21	0.41
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.75	0.41
1:B:318:THR:O	1:B:319:HIS:C	2.58	0.41
1:A:5:PHE:O	1:A:145:VAL:HA	2.21	0.41
1:A:395:VAL:O	1:A:395:VAL:CG1	2.67	0.41
1:A:399:THR:HB	1:A:417:LEU:HB3	2.03	0.41
1:B:445:ASN:HA	2:B:491:HOH:O	2.19	0.41
1:A:49:VAL:O	1:A:50:CYS:C	2.59	0.41
1:A:192:HIS:ND1	1:A:203:THR:OG1	2.48	0.41
1:A:299:LEU:CD2	1:A:352:LEU:CD1	2.91	0.41
1:B:332:LYS:HB3	1:B:333:PRO:HD2	2.02	0.41
1:A:264:ASN:OD1	1:A:264:ASN:N	2.47	0.41
1:A:344:GLY:H	1:A:347:GLU:CD	2.24	0.41
1:A:365:VAL:HG11	1:A:371:MET:SD	2.61	0.41
1:A:332:LYS:HG3	1:A:336:PHE:CD2	2.56	0.40
1:A:27:ASN:O	1:A:28:ALA:C	2.60	0.40
1:A:193:PHE:O	1:A:202:VAL:HG12	2.21	0.40
1:A:299:LEU:HD23	1:A:352:LEU:HD13	1.93	0.40
1:B:46:VAL:HG22	1:B:57:TRP:CZ3	2.56	0.40
1:A:404:ALA:HB3	1:A:413:LYS:HB3	2.03	0.40
1:B:360:SER:HB2	2:B:464:HOH:O	2.20	0.40
1:B:416:ILE:HD11	1:B:439:LYS:CD	2.47	0.40
1:A:16:GLN:HG2	1:A:135:TYR:HD1	1.84	0.40
1:A:395:VAL:O	1:A:395:VAL:HG13	2.21	0.40
1:A:416:ILE:C	1:A:416:ILE:HD12	2.41	0.40
1:B:243:PHE:HA	1:B:244:PRO:HD2	1.93	0.40
1:A:104:GLN:HG3	2:A:484:HOH:O	2.22	0.40
1:A:109:ILE:HD13	1:A:161:LEU:HD21	2.04	0.40
1:A:424:ALA:O	1:A:426:ASP:N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:O	2:B:463:HOH:O[2_556]	2.18	0.02

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	406/481 (84%)	352 (87%)	45 (11%)	9 (2%)	6 12
1	B	401/481 (83%)	346 (86%)	45 (11%)	10 (2%)	5 9
All	All	807/962 (84%)	698 (86%)	90 (11%)	19 (2%)	6 10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO
1	A	73	CYS
1	A	182	GLY
1	B	208	SER
1	B	212	ASP
1	B	425	GLU
1	A	2	ASP
1	A	78	ARG
1	A	264	ASN
1	B	196	PRO
1	B	198	LYS
1	B	314	ARG
1	A	217	ALA
1	B	442	ASP
1	A	154	TRP
1	B	22	GLU
1	B	334	ALA
1	B	335	THR
1	A	77	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	366/424 (86%)	291 (80%)	75 (20%)	1 2
1	B	360/424 (85%)	306 (85%)	54 (15%)	3 5
All	All	726/848 (86%)	597 (82%)	129 (18%)	2 3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	ILE
1	A	16	GLN
1	A	17	LEU
1	A	30	ARG
1	A	33	LEU
1	A	36	LEU
1	A	39	LYS
1	A	40	LEU
1	A	41	SER
1	A	46	VAL
1	A	47	LEU
1	A	57	TRP
1	A	61	ASP
1	A	70	SER
1	A	74	LYS
1	A	76	VAL
1	A	78	ARG
1	A	80	ILE
1	A	113	LEU
1	A	116	SER
1	A	134	HIS
1	A	135	TYR
1	A	145	VAL
1	A	147	SER
1	A	151	GLU
1	A	161	LEU
1	A	178	ARG
1	A	180	MET
1	A	183	THR
1	A	186	VAL
1	A	199	LYS
1	A	201	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	HIS
1	A	238	ILE
1	A	249	LYS
1	A	261	SER
1	A	264	ASN
1	A	266	GLU
1	A	273	VAL
1	A	276	THR
1	A	279	TYR
1	A	285	ASP
1	A	294	SER
1	A	297	ARG
1	A	299	LEU
1	A	304	SER
1	A	307	ARG
1	A	314	ARG
1	A	316	ILE
1	A	322	ILE
1	A	326	LEU
1	A	335	THR
1	A	343	ILE
1	A	345	SER
1	A	352	LEU
1	A	360	SER
1	A	361	LYS
1	A	363	LEU
1	A	383	GLN
1	A	384	ASN
1	A	385	VAL
1	A	390	MET
1	A	395	VAL
1	A	400	ILE
1	A	409	THR
1	A	413	LYS
1	A	426	ASP
1	A	431	LEU
1	A	439	LYS
1	A	446	LYS
1	A	449	TYR
1	A	452	LEU
1	A	459	ASN
1	A	461	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	15	PHE
1	B	17	LEU
1	B	21	LYS
1	B	29	LEU
1	B	33	LEU
1	B	42	SER
1	B	46	VAL
1	B	52	SER
1	B	59	ASN
1	B	61	ASP
1	B	66	GLU
1	B	67	LEU
1	B	69	ASP
1	B	103	THR
1	B	112	MET
1	B	135	TYR
1	B	156	LYS
1	B	159	LYS
1	B	160	LEU
1	B	165	ILE
1	B	166	LEU
1	B	168	GLN
1	B	169	LEU
1	B	170	VAL
1	B	198	LYS
1	B	199	LYS
1	B	202	VAL
1	B	208	SER
1	B	210	ILE
1	B	219	ARG
1	B	225	LEU
1	B	238	ILE
1	B	266	GLU
1	B	274	GLN
1	B	276	THR
1	B	279	TYR
1	B	299	LEU
1	B	304	SER
1	B	312	THR
1	B	326	LEU
1	B	332	LYS
1	B	362	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	365	VAL
1	B	367	GLN
1	B	390	MET
1	B	396	LEU
1	B	400	ILE
1	B	411	GLN
1	B	416	ILE
1	B	422	THR
1	B	431	LEU
1	B	439	LYS
1	B	445	ASN
1	B	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	59	ASN
1	A	105	GLN
1	A	108	ASN
1	A	200	ASN
1	A	214	GLN
1	A	284	GLN
1	A	383	GLN
1	A	445	ASN
1	B	31	GLN
1	B	104	GLN
1	B	194	GLN
1	B	200	ASN
1	B	274	GLN
1	B	280	HIS
1	B	284	GLN
1	B	354	GLN
1	B	367	GLN
1	B	374	GLN
1	B	383	GLN
1	B	445	ASN
1	B	459	ASN

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 monosaccharides 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	416/481 (86%)	-0.29	9 (2%)	62	56	5, 36, 81, 119	0
1	B	411/481 (85%)	-0.24	9 (2%)	62	56	5, 40, 83, 118	0
All	All	827/962 (85%)	-0.26	18 (2%)	62	56	5, 38, 82, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	THR	5.8
1	A	263	PRO	5.6
1	B	135	TYR	4.7
1	A	59	ASN	4.1
1	B	115	ILE	4.0
1	A	67	LEU	3.3
1	A	103	THR	2.9
1	B	186	VAL	2.5
1	B	209	GLY	2.4
1	A	431	LEU	2.3
1	A	260	LEU	2.3
1	B	211	PRO	2.3
1	B	212	ASP	2.3
1	B	208	SER	2.2
1	B	116	SER	2.2
1	B	287	ILE	2.1
1	A	268	SER	2.0
1	A	115	ILE	2.0

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

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.