



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:00 PM UTC

PDB ID : 3OQC / pdb_00003oqc
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

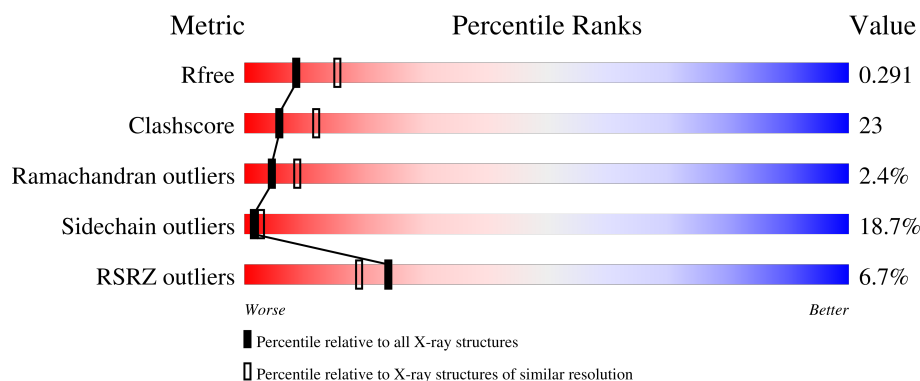
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	6% 46% 30% 10% 14%
1	B	481	5% 47% 30% 9% 15%

2 Entry composition

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

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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

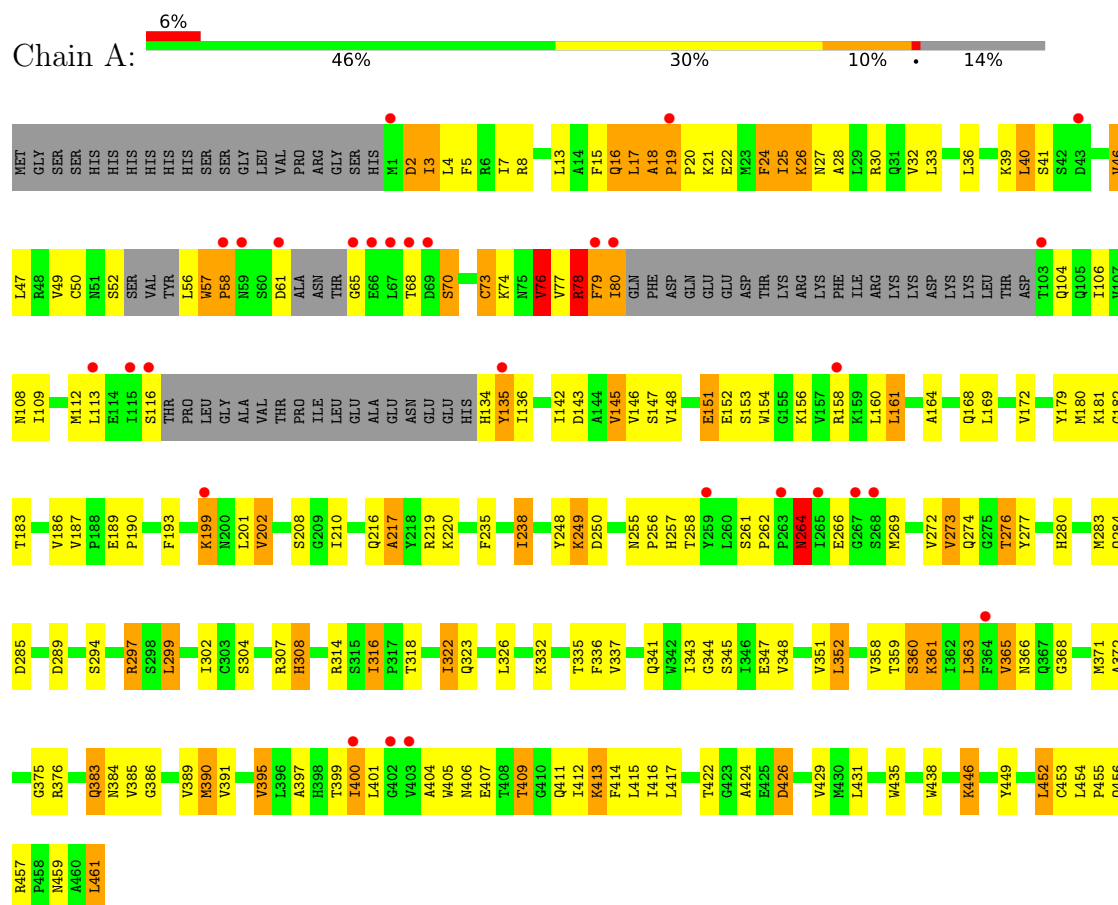
- Molecule 2 is water.

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

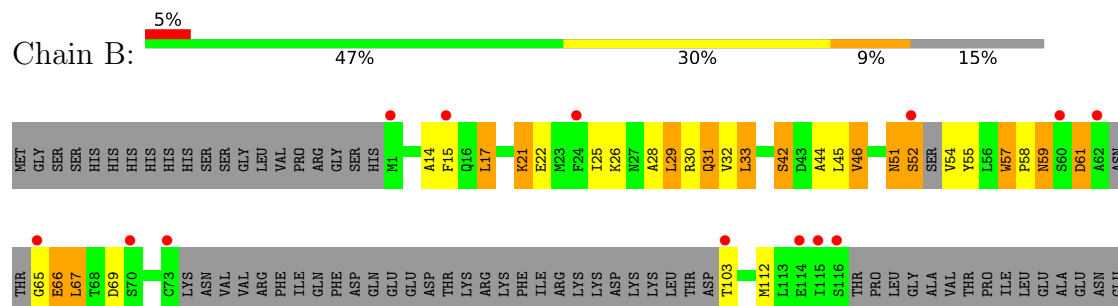
3 Residue-property plots

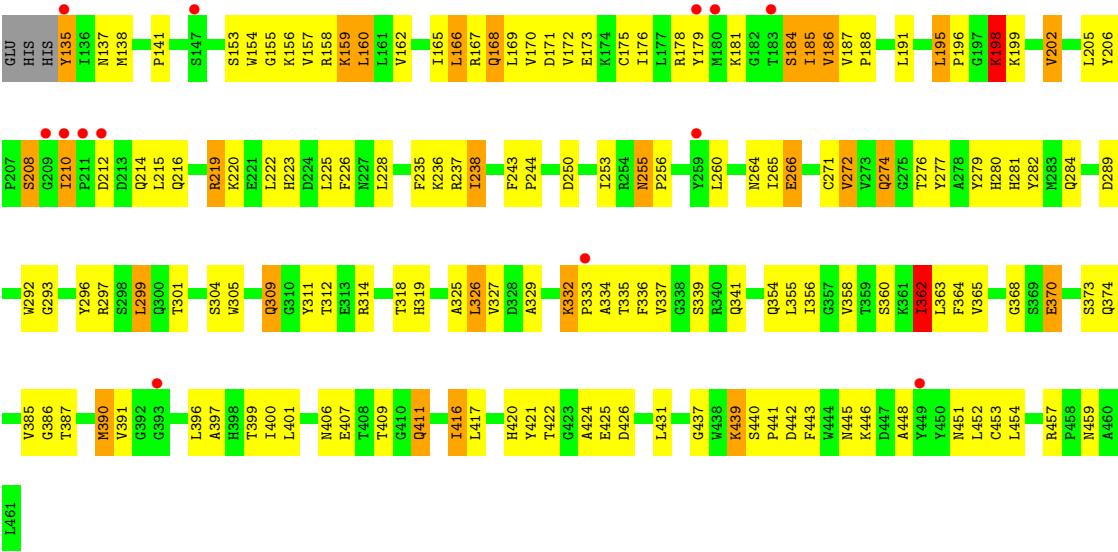
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Ufm1-specific protease 2





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.94%)	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)	0.32 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.93	2/3409 (0.1%)	1.19	17/4627 (0.4%)
1	B	0.88	1/3361 (0.0%)	1.17	14/4564 (0.3%)
All	All	0.90	3/6770 (0.0%)	1.18	31/9191 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ALA	CA-CB	-6.89	1.42	1.53
1	A	65	GLY	N-CA	6.79	1.56	1.45
1	B	271	CYS	CA-C	-6.18	1.46	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	LEU	CA-C-N	9.03	131.13	119.84
1	B	195	LEU	C-N-CA	9.03	131.13	119.84
1	B	255	ASN	CA-C-N	8.35	128.04	119.19
1	B	255	ASN	C-N-CA	8.35	128.04	119.19
1	A	79	PHE	N-CA-C	8.20	122.61	108.02
1	A	26	LYS	N-CA-C	-8.14	102.10	110.97
1	A	19	PRO	N-CA-C	7.64	120.03	110.70
1	B	440	SER	CA-C-N	-7.29	112.19	119.56
1	B	440	SER	C-N-CA	-7.29	112.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	TRP	N-CA-C	-6.49	105.49	113.41
1	A	18	ALA	CA-C-N	6.37	126.94	120.38
1	A	18	ALA	C-N-CA	6.37	126.94	120.38
1	B	186	VAL	N-CA-C	6.25	116.63	107.37
1	A	136	ILE	N-CA-C	6.20	117.53	108.53
1	A	366	ASN	N-CA-C	6.03	119.11	111.69
1	B	51	ASN	N-CA-C	5.60	119.31	111.74
1	A	235	PHE	N-CA-C	5.60	117.16	110.44
1	A	24	PHE	N-CA-C	5.55	120.05	113.12
1	A	187	VAL	CA-C-N	-5.46	114.36	120.14
1	A	187	VAL	C-N-CA	-5.46	114.36	120.14
1	A	358	VAL	N-CA-C	5.46	116.84	108.71
1	B	272	VAL	CB-CA-C	5.43	118.62	111.19
1	B	399	THR	CA-C-N	-5.36	115.37	122.98
1	B	399	THR	C-N-CA	-5.36	115.37	122.98
1	A	210	ILE	CB-CA-C	5.35	115.32	110.13
1	B	250	ASP	N-CA-C	-5.30	105.88	114.09
1	A	269	MET	N-CA-C	-5.26	101.12	109.59
1	B	264	ASN	N-CA-C	5.25	119.54	113.18
1	A	76	VAL	CB-CA-C	-5.23	105.01	111.70
1	A	308	HIS	N-CA-C	5.13	116.56	111.07
1	B	362	ILE	N-CA-C	5.10	115.47	108.12

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 ⓘ

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	171	1
1	B	3281	0	3243	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	0	15	0
2	B	54	0	0	10	1
All	All	6716	0	6540	305	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 23.

All (305) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:322:ILE:HG13	1:A:323:GLN:N	2.09	0.67
1:B:238:ILE:O	1:B:238:ILE:HG13	1.92	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
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:A:449:TYR:CD1	1:A:449:TYR:C	2.76	0.63
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:B:219:ARG:HD3	1:B:235:PHE:C	2.25	0.61
1:A:372:ALA:HA	1:A:412:ILE:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:138:MET:HE2	1:B:185:ILE:HG12	1.87	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
1:B:441:PRO:C	1:B:443:PHE:H	2.14	0.56
1:B:445:ASN:C	1:B:445:ASN:HD22	2.12	0.56
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: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:B:166:LEU:O	1:B:167:ARG:C	2.50	0.55
1:A:216:GLN:CA	2:A:476:HOH:O	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:ASP:CG	1:A:297:ARG:NH1	2.66	0.53
1:A:52:SER:CA	1:A:79:PHE:HD2	2.21	0.53
1:A:151:GLU:O	1:A:152:GLU:C	2.52	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:277:TYR:CD2	1:B:277:TYR:C	2.87	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
1:B:171:ASP:HB3	1:B:205:LEU:HD12	1.92	0.51
1:A:449:TYR:C	1:A:449:TYR:HD1	2.19	0.51
1:A:52:SER:C	1:A:79:PHE:CE2	2.89	0.51
1:A:453:CYS:C	1:A:454:LEU:HD12	2.35	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:A:219:ARG:NH1	1:A:461:LEU:C	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASN:CG	1:B:409:THR:HG22	2.36	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:O	1:A:217:ALA:C	2.54	0.50
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:A:46:VAL:HG22	1:A:112:MET:HE3	1.94	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: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:52:SER:C	1:A:79:PHE:CD2	2.90	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: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: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:A:289:ASP:CG	1:A:297:ARG:HH11	2.23	0.47
1:B:141:PRO:HD3	1:B:187:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:VAL:O	1:A:78:ARG:N	2.48	0.46
1:B:336:PHE:O	1:B:339:SER:HB2	2.15	0.46
1:A:277:TYR:C	1:A:277:TYR:CD2	2.93	0.46
1:A:284:GLN:HB2	1:A:297:ARG:NH2	2.31	0.46
1:B:318:THR:O	1:B:319:HIS:C	2.58	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:391:VAL:HG12	1:A:452:LEU:CD2	2.45	0.46
1:A:49:VAL:O	1:A:50:CYS:C	2.59	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:344:GLY:H	1:A:347:GLU:CD	2.24	0.45
1:A:56:LEU:HG	2:A:489:HOH:O	2.16	0.45
1:A:27:ASN:O	1:A:28:ALA:C	2.60	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:A:416:ILE:HD12	1:A:416:ILE:C	2.41	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:248:TYR:O	1:A:249:LYS:C	2.59	0.44
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: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:390:MET:HE1	1:B:397:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:451:ASN:C	1:B:452:LEU:HD12	2.43	0.43
1:A:112:MET:HE3	1:A:112:MET:HB2	1.76	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:445:ASN:C	1:B:445:ASN:ND2	2.71	0.43
1:A:46:VAL:HG22	1:A:112:MET:CE	2.49	0.43
1:A:179:TYR:O	1:A:180:MET:C	2.61	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: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:76:VAL:C	1:A:78:ARG:N	2.77	0.42
1:A:249:LYS:CD	1:A:249:LYS:H	2.31	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:373:SER:C	1:B:374:GLN:HE21	2.28	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:326:LEU:O	1:B:327:VAL:C	2.62	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: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:B:186:VAL:O	1:B:188:PRO:HD3	2.19	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD2	1:A:250:ASP:C	2.62	0.41
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.75	0.41
1:B:299:LEU:HD23	1:B:299:LEU:C	2.45	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:236:LYS:O	1:B:237:ARG:C	2.63	0.41
1:B:445:ASN:HA	2:B:491:HOH:O	2.19	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:365:VAL:HG11	1:A:371:MET:SD	2.61	0.41
1:B:31:GLN:O	1:B:32:VAL:C	2.64	0.41
1:B:445:ASN:HD22	1:B:446:LYS:N	2.17	0.41
1:A:332:LYS:HG3	1:A:336:PHE:CD2	2.56	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:B:337:VAL:C	1:B:339:SER:H	2.28	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: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%)	5	10
1	B	401/481 (83%)	346 (86%)	45 (11%)	10 (2%)	4	8
All	All	807/962 (84%)	698 (86%)	90 (11%)	19 (2%)	4	9

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%)	299 (83%)	61 (17%)	2	4
All	All	726/848 (86%)	590 (81%)	136 (19%)	1	3

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	ILE
1	A	7	ILE
1	A	13	LEU
1	A	16	GLN
1	A	17	LEU
1	A	22	GLU
1	A	25	ILE
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	183	THR
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	199	LYS
1	A	201	LEU
1	A	202	VAL
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	285	ASP
1	A	294	SER
1	A	297	ARG
1	A	299	LEU
1	A	314	ARG
1	A	316	ILE
1	A	322	ILE
1	A	326	LEU
1	A	335	THR
1	A	337	VAL
1	A	343	ILE
1	A	345	SER
1	A	352	LEU
1	A	359	THR
1	A	360	SER
1	A	361	LYS
1	A	363	LEU
1	A	365	VAL
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	446	LYS
1	A	452	LEU
1	A	459	ASN
1	A	461	LEU

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Mol	Chain	Res	Type
1	B	15	PHE
1	B	17	LEU
1	B	21	LYS
1	B	29	LEU
1	B	31	GLN
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	184	SER
1	B	185	ILE
1	B	198	LYS
1	B	199	LYS
1	B	202	VAL
1	B	208	SER
1	B	210	ILE
1	B	214	GLN
1	B	219	ARG
1	B	225	LEU
1	B	238	ILE
1	B	253	ILE
1	B	266	GLU
1	B	272	VAL
1	B	274	GLN
1	B	276	THR
1	B	299	LEU

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Mol	Chain	Res	Type
1	B	301	THR
1	B	304	SER
1	B	309	GLN
1	B	312	THR
1	B	326	LEU
1	B	332	LYS
1	B	354	GLN
1	B	362	ILE
1	B	365	VAL
1	B	370	GLU
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	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	105	GLN
1	A	108	ASN
1	A	200	ASN
1	A	214	GLN
1	A	216	GLN
1	A	274	GLN
1	A	284	GLN
1	A	341	GLN
1	A	383	GLN
1	A	398	HIS
1	A	445	ASN
1	B	104	GLN
1	B	194	GLN
1	B	200	ASN
1	B	239	ASN
1	B	274	GLN
1	B	280	HIS
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	367	GLN
1	B	374	GLN
1	B	383	GLN
1	B	445	ASN
1	B	459	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 oligosaccharides 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

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, 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	416/481 (86%)	0.21	29 (6%) 22 18	5, 36, 81, 119	0
1	B	411/481 (85%)	0.25	26 (6%) 26 20	5, 40, 83, 118	0
All	All	827/962 (85%)	0.23	55 (6%) 24 19	5, 38, 82, 119	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	LEU	5.7
1	A	65	GLY	5.1
1	A	59	ASN	4.9
1	A	263	PRO	4.9
1	A	115	ILE	4.8
1	B	135	TYR	4.3
1	B	73	CYS	4.2
1	B	62	ALA	4.0
1	A	265	ILE	3.8
1	A	135	TYR	3.7
1	B	115	ILE	3.7
1	B	210	ILE	3.7
1	A	402	GLY	3.5
1	B	52	SER	3.5
1	A	259	TYR	3.4
1	A	268	SER	3.4
1	A	364	PHE	3.3
1	A	400	ILE	3.2
1	B	393	GLY	3.1
1	A	61	ASP	3.1
1	B	209	GLY	3.1
1	B	449	TYR	2.9
1	B	114	GLU	2.8
1	B	1	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	PRO	2.7
1	B	103	THR	2.6
1	A	80	ILE	2.6
1	A	68	THR	2.6
1	A	103	THR	2.6
1	A	116	SER	2.5
1	B	259	TYR	2.5
1	A	113	LEU	2.5
1	A	158	ARG	2.4
1	B	116	SER	2.4
1	A	403	VAL	2.4
1	B	24	PHE	2.3
1	A	43	ASP	2.3
1	B	60	SER	2.3
1	B	147	SER	2.3
1	B	179	TYR	2.3
1	A	58	PRO	2.3
1	B	212	ASP	2.3
1	B	65	GLY	2.3
1	A	1	MET	2.3
1	B	211	PRO	2.2
1	B	70	SER	2.2
1	A	79	PHE	2.2
1	A	66	GLU	2.2
1	B	180	MET	2.1
1	B	15	PHE	2.1
1	A	199	LYS	2.0
1	A	69	ASP	2.0
1	B	183	THR	2.0
1	B	333	PRO	2.0
1	A	267	GLY	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 oligosaccharides 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.