



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:22 PM GMT

PDB ID : 2IO2
Title : Crystal structure of human Senp2 in complex with RanGAP1-SUMO-1
Authors : Reverter, D.; Lima, C.D.
Deposited on : 2006-10-09
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

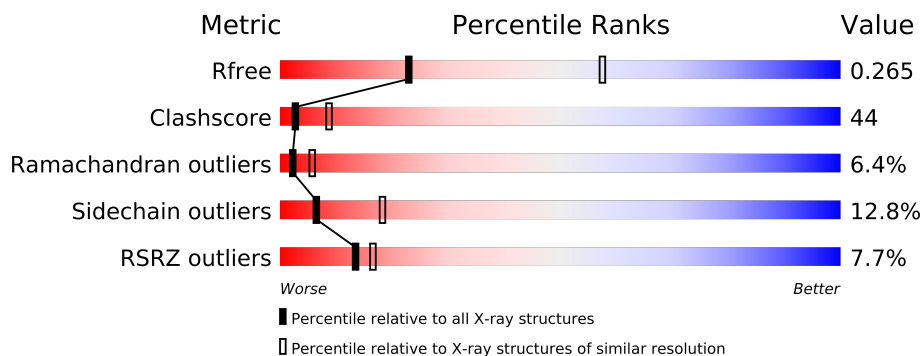
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	232	
2	B	82	
3	C	172	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3696 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sentrin-specific protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1876	1207	327	332	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	GLY	-	CLONING ARTIFACT	UNP Q9HC62
A	359	SER	-	CLONING ARTIFACT	UNP Q9HC62
A	360	HIS	-	CLONING ARTIFACT	UNP Q9HC62
A	361	MET	-	CLONING ARTIFACT	UNP Q9HC62
A	362	ALA	-	CLONING ARTIFACT	UNP Q9HC62
A	363	SER	-	CLONING ARTIFACT	UNP Q9HC62
A	548	SER	CYS	ENGINEERED	UNP Q9HC62

- Molecule 2 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			608	380	106	118	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	CLONING ARTIFACT	UNP P63165
B	17	GLY	-	CLONING ARTIFACT	UNP P63165

- Molecule 3 is a protein called Ran GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1204	775	199	225	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	416	SER	-	CLONING ARTIFACT	UNP P46060
C	417	LEU	-	CLONING ARTIFACT	UNP P46060
C	573	SER	CYS	ENGINEERED	UNP P46060

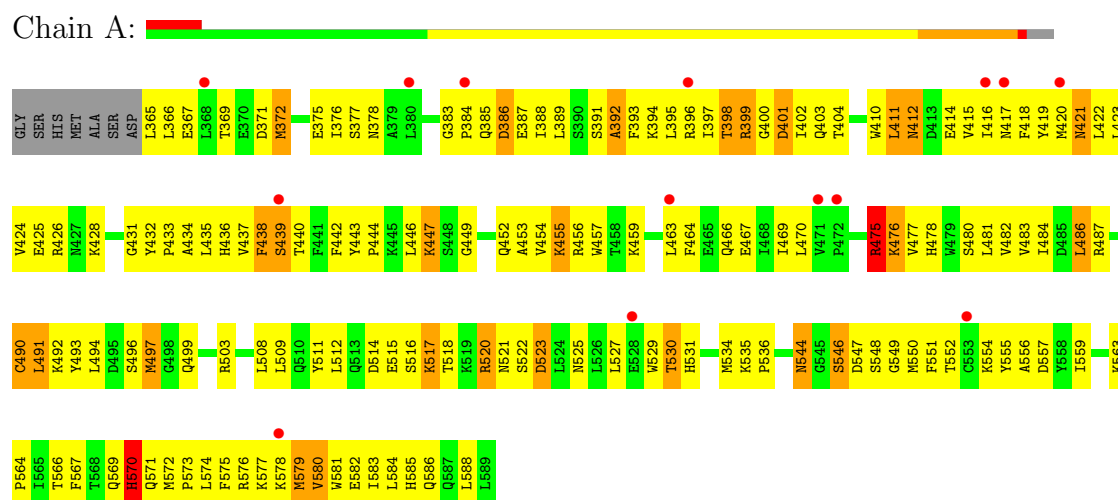
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0

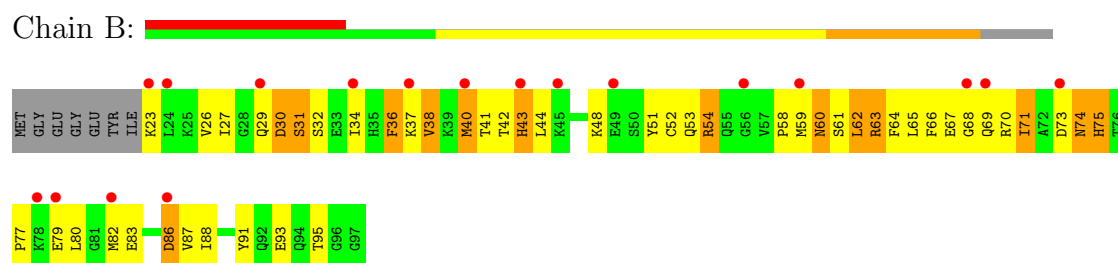
3 Residue-property plots

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

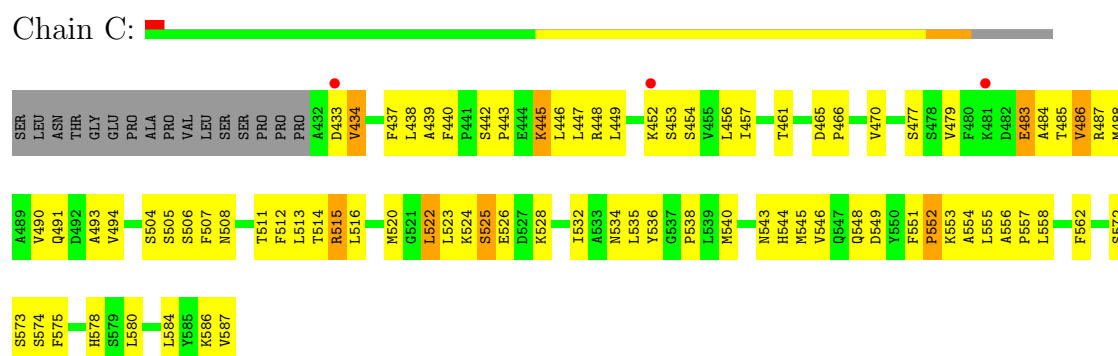
• Molecule 1: Sentrin-specific protease 2



• Molecule 2: Small ubiquitin-related modifier 1



• Molecule 3: Ran GTPase-activating protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.96Å 163.96Å 77.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.94 – 2.90 28.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (14.94-2.90) 96.8 (28.40-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.301 0.261 , 0.265	Depositor DCC
R_{free} test set	671 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 25.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	4 of 13667 reflections (0.029%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3696	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.39	0/1922	0.68	1/2589 (0.0%)
2	B	0.37	0/617	0.66	0/822
3	C	0.40	0/1227	0.67	0/1661
All	All	0.39	0/3766	0.67	1/5072 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	N-CA-C	-6.99	92.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1892	198	0
2	B	608	0	606	62	0
3	C	1204	0	1239	77	0
4	A	5	0	0	0	1
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	3696	0	3737	325	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (325) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:23:LYS:HA	2:B:37:LYS:HG2	1.34	1.09
1:A:464:PHE:HA	1:A:486:LEU:HD11	1.52	0.92
3:C:543:ASN:O	3:C:546:VAL:HG22	1.75	0.87
3:C:453:SER:O	3:C:457:ILE:HG12	1.76	0.86
1:A:577:LYS:O	1:A:580:VAL:HG13	1.77	0.84
1:A:490:CYS:HB2	1:A:530:THR:HG22	1.59	0.83
3:C:442:SER:HB3	3:C:445:LYS:HB2	1.57	0.83
2:B:83:GLU:O	2:B:86:ASP:HB2	1.81	0.81
1:A:475:ARG:NH2	1:A:499:GLN:NE2	2.28	0.80
2:B:36:PHE:O	2:B:37:LYS:HG3	1.82	0.79
3:C:490:VAL:O	3:C:494:VAL:HG23	1.83	0.78
2:B:66:PHE:CZ	2:B:82:MET:HG3	2.19	0.78
1:A:401:ASP:O	1:A:404:THR:HG23	1.83	0.77
1:A:426:ARG:HD2	1:A:426:ARG:O	1.86	0.75
1:A:476:LYS:HG3	1:A:477:VAL:HG13	1.68	0.75
2:B:66:PHE:HB2	2:B:71:ILE:HD11	1.69	0.75
1:A:469:ILE:HG22	1:A:484:ILE:HD13	1.70	0.73
3:C:466:PRO:O	3:C:470:VAL:HG23	1.89	0.72
3:C:516:LEU:HD21	3:C:520:MET:HE1	1.71	0.72
1:A:481:LEU:HD12	1:A:482:VAL:N	2.05	0.71
1:A:481:LEU:HB2	1:A:552:THR:HG23	1.71	0.71
1:A:544:ASN:C	1:A:544:ASN:HD22	1.93	0.71
3:C:449:LEU:CB	3:C:453:SER:HB3	2.20	0.71
1:A:525:ASN:HD21	1:A:527:LEU:HB2	1.55	0.71
1:A:454:VAL:O	1:A:457:TRP:HB2	1.91	0.70
1:A:375:GLU:HA	1:A:378:ASN:ND2	2.06	0.70
1:A:388:ILE:HG12	1:A:396:ARG:HD3	1.72	0.70
1:A:395:LEU:CD2	2:B:70:ARG:HD3	2.22	0.70
1:A:578:LYS:O	1:A:582:GLU:HG3	1.91	0.70
1:A:449:GLY:O	1:A:453:ALA:HB3	1.91	0.70
1:A:463:LEU:HG	1:A:469:ILE:HD11	1.74	0.70
1:A:494:LEU:HG	1:A:534:MET:HG3	1.71	0.70
1:A:388:ILE:HD12	1:A:388:ILE:H	1.57	0.70
1:A:579:MET:O	1:A:583:ILE:HG13	1.92	0.69
3:C:580:LEU:O	3:C:584:LEU:HD23	1.93	0.69
3:C:556:ALA:N	3:C:557:PRO:HD2	2.08	0.68
1:A:491:LEU:CD1	1:A:531:HIS:HB3	2.24	0.68
1:A:411:LEU:HD13	1:A:415:VAL:HG11	1.74	0.68
3:C:434:VAL:CG1	3:C:457:ILE:HD13	2.24	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:476:LYS:CG	1:A:477:VAL:HG13	2.24	0.68
3:C:552:PRO:HG2	3:C:555:LEU:HD12	1.75	0.68
1:A:573:PRO:O	1:A:576:ARG:HB2	1.93	0.68
3:C:470:VAL:HG22	3:C:512:PHE:CD1	2.28	0.67
1:A:399:ARG:O	1:A:403:GLN:HG2	1.94	0.67
3:C:449:LEU:HB2	3:C:453:SER:HB3	1.77	0.67
1:A:544:ASN:ND2	1:A:546:SER:H	1.93	0.67
1:A:554:LYS:HE3	1:A:575:PHE:CD1	2.29	0.67
3:C:580:LEU:HD23	3:C:584:LEU:HD23	1.75	0.67
2:B:82:MET:CE	2:B:88:ILE:HD11	2.26	0.66
2:B:27:ILE:HD12	2:B:27:ILE:H	1.60	0.66
2:B:66:PHE:CE1	2:B:67:GLU:HG2	2.30	0.66
1:A:484:ILE:HG23	1:A:491:LEU:HD23	1.77	0.65
3:C:586:LYS:O	3:C:587:VAL:HG23	1.96	0.65
1:A:466:GLN:O	1:A:486:LEU:HD13	1.96	0.65
1:A:376:ILE:HG12	1:A:580:VAL:HG21	1.79	0.65
1:A:418:PHE:CD2	1:A:583:ILE:HG23	2.32	0.65
1:A:554:LYS:HE3	1:A:575:PHE:HD1	1.62	0.65
2:B:66:PHE:CD1	2:B:67:GLU:HG2	2.32	0.65
1:A:398:THR:O	1:A:402:ILE:HG22	1.96	0.65
1:A:447:LYS:HD2	1:A:503:ARG:NH2	2.12	0.65
1:A:391:SER:O	1:A:392:ALA:HB2	1.98	0.64
3:C:448:ARG:HH11	3:C:448:ARG:HG3	1.62	0.64
1:A:383:GLY:HA3	1:A:399:ARG:HH12	1.63	0.63
1:A:572:MET:HA	1:A:575:PHE:HD2	1.64	0.63
2:B:34:ILE:HD12	2:B:51:TYR:CE1	2.33	0.63
1:A:525:ASN:ND2	1:A:527:LEU:HB2	2.14	0.63
2:B:23:LYS:CA	2:B:37:LYS:HG2	2.21	0.63
1:A:412:ASN:HD21	1:A:415:VAL:HB	1.64	0.63
1:A:508:LEU:O	1:A:511:TYR:HB3	1.99	0.62
1:A:525:ASN:O	1:A:529:TRP:HD1	1.82	0.62
1:A:366:LEU:HD13	1:A:578:LYS:NZ	2.14	0.62
1:A:371:ASP:O	1:A:375:GLU:HG3	2.00	0.62
1:A:544:ASN:HD21	1:A:547:ASP:H	1.47	0.62
2:B:37:LYS:O	2:B:38:VAL:HG13	2.00	0.62
3:C:445:LYS:NZ	3:C:445:LYS:HB2	2.15	0.62
1:A:412:ASN:HD21	1:A:415:VAL:H	1.48	0.61
1:A:411:LEU:HD23	1:A:411:LEU:N	2.15	0.61
1:A:470:LEU:CD1	1:A:556:ALA:HB1	2.30	0.61
1:A:484:ILE:HA	1:A:491:LEU:HB3	1.82	0.61
1:A:424:VAL:HA	1:A:435:LEU:HD23	1.82	0.61
1:A:412:ASN:ND2	1:A:415:VAL:H	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:393:PHE:O	1:A:394:LYS:HB2	2.00	0.60
3:C:442:SER:HB3	3:C:445:LYS:CB	2.28	0.60
1:A:467:GLU:HB3	1:A:487:ARG:HD3	1.83	0.60
1:A:514:ASP:O	1:A:518:THR:HB	2.00	0.60
2:B:27:ILE:HD13	2:B:87:VAL:HG13	1.84	0.60
1:A:475:ARG:NH2	1:A:499:GLN:CD	2.55	0.59
1:A:483:VAL:HG11	1:A:559:ILE:HG21	1.82	0.59
2:B:36:PHE:O	2:B:37:LYS:CG	2.49	0.59
1:A:436:HIS:HB3	1:A:469:ILE:HG12	1.83	0.59
1:A:499:GLN:NE2	3:C:515:ARG:NH2	2.50	0.59
1:A:443:TYR:HB3	1:A:444:PRO:HD3	1.84	0.59
1:A:412:ASN:HD22	1:A:412:ASN:C	2.06	0.59
1:A:432:TYR:HB3	1:A:433:PRO:HD2	1.85	0.59
2:B:82:MET:SD	2:B:88:ILE:HD11	2.43	0.59
1:A:372:MET:HB3	1:A:581:TRP:HE1	1.68	0.58
1:A:476:LYS:HG3	1:A:477:VAL:CG1	2.34	0.58
2:B:66:PHE:CE2	2:B:82:MET:HG3	2.37	0.58
1:A:491:LEU:HD12	1:A:531:HIS:HB3	1.86	0.58
1:A:469:ILE:CG2	1:A:484:ILE:HD13	2.34	0.57
1:A:490:CYS:CB	1:A:530:THR:HG22	2.32	0.57
3:C:520:MET:O	3:C:522:LEU:HD23	2.04	0.57
3:C:449:LEU:HB3	3:C:453:SER:HB3	1.84	0.57
1:A:411:LEU:HD23	1:A:411:LEU:H	1.69	0.57
3:C:573:SER:C	3:C:575:PHE:H	2.08	0.57
1:A:436:HIS:HB2	1:A:466:GLN:HG3	1.85	0.57
1:A:412:ASN:ND2	1:A:415:VAL:HB	2.19	0.57
2:B:54:ARG:H	2:B:54:ARG:HD3	1.70	0.57
1:A:454:VAL:HA	1:A:457:TRP:CD1	2.39	0.56
1:A:520:ARG:O	1:A:522:SER:N	2.38	0.56
1:A:385:GLN:HE21	1:A:400:GLY:HA2	1.70	0.56
3:C:486:VAL:O	3:C:490:VAL:HG23	2.06	0.56
1:A:536:PRO:HB2	3:C:508:ASN:ND2	2.21	0.56
2:B:52:CYS:SG	2:B:59:MET:HB2	2.46	0.56
1:A:366:LEU:HD13	1:A:578:LYS:HZ2	1.71	0.55
1:A:447:LYS:HD2	1:A:503:ARG:HH21	1.71	0.55
3:C:448:ARG:HH11	3:C:448:ARG:CG	2.18	0.55
1:A:491:LEU:O	1:A:531:HIS:HA	2.06	0.55
3:C:434:VAL:HG12	3:C:457:ILE:HD13	1.89	0.55
1:A:470:LEU:HD11	1:A:556:ALA:HB1	1.89	0.55
1:A:520:ARG:C	1:A:522:SER:H	2.10	0.55
1:A:569:GLN:O	1:A:571:GLN:N	2.35	0.54
1:A:418:PHE:O	1:A:421:ASN:N	2.33	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:484:ILE:HD12	1:A:484:ILE:N	2.23	0.54
1:A:459:LYS:NZ	2:B:69:GLN:HE21	2.05	0.54
2:B:62:LEU:C	2:B:63:ARG:HD2	2.28	0.54
2:B:59:MET:HG2	2:B:60:ASN:N	2.22	0.54
1:A:480:SER:HB3	1:A:493:TYR:HE1	1.73	0.54
2:B:23:LYS:HE2	2:B:37:LYS:HZ2	1.72	0.54
1:A:432:TYR:HB3	1:A:433:PRO:CD	2.38	0.53
3:C:545:MET:HG2	3:C:551:PHE:CE1	2.42	0.53
1:A:375:GLU:HA	1:A:378:ASN:HD22	1.72	0.53
1:A:484:ILE:HD12	1:A:484:ILE:H	1.73	0.52
2:B:75:HIS:CD2	2:B:80:LEU:HG	2.45	0.52
1:A:452:GLN:HG3	1:A:453:ALA:N	2.23	0.52
1:A:385:GLN:NE2	1:A:403:GLN:HG3	2.23	0.52
1:A:419:TYR:CD1	1:A:579:MET:SD	3.02	0.52
1:A:512:LEU:O	1:A:515:GLU:N	2.42	0.52
1:A:420:MET:O	1:A:437:VAL:HG21	2.09	0.52
3:C:505:SER:C	3:C:507:PHE:H	2.12	0.52
3:C:516:LEU:CD2	3:C:520:MET:HE1	2.38	0.52
3:C:535:LEU:O	3:C:536:TYR:C	2.48	0.52
1:A:419:TYR:OH	1:A:557:ASP:HB2	2.10	0.52
1:A:419:TYR:CE1	1:A:588:LEU:HD21	2.45	0.52
3:C:580:LEU:HD23	3:C:584:LEU:CD2	2.40	0.52
1:A:480:SER:HB3	1:A:493:TYR:CE1	2.44	0.51
1:A:376:ILE:HD11	1:A:580:VAL:HG13	1.91	0.51
3:C:572:SER:O	3:C:575:PHE:HB3	2.10	0.51
3:C:488:MET:HA	3:C:491:GLN:HE21	1.75	0.51
2:B:64:PHE:N	2:B:64:PHE:CD1	2.79	0.51
3:C:528:LYS:O	3:C:532:ILE:HG13	2.11	0.51
2:B:79:GLU:HG2	2:B:79:GLU:O	2.11	0.51
1:A:483:VAL:HG11	1:A:559:ILE:CG2	2.40	0.51
3:C:452:LYS:O	3:C:456:LEU:HB2	2.11	0.51
1:A:386:ASP:O	1:A:388:ILE:HD12	2.10	0.51
1:A:391:SER:O	1:A:392:ALA:CB	2.58	0.51
1:A:366:LEU:HB2	1:A:578:LYS:HZ1	1.76	0.50
2:B:65:LEU:HD12	2:B:65:LEU:N	2.26	0.50
1:A:464:PHE:N	1:A:464:PHE:CD1	2.79	0.50
1:A:544:ASN:HD22	1:A:546:SER:H	1.60	0.50
1:A:395:LEU:HD22	2:B:70:ARG:HD3	1.93	0.50
1:A:517:LYS:HB2	1:A:523:ASP:HA	1.94	0.50
3:C:543:ASN:O	3:C:544:HIS:C	2.49	0.50
3:C:543:ASN:O	3:C:546:VAL:CG2	2.54	0.50
1:A:376:ILE:CG2	1:A:377:SER:N	2.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:88:ILE:O	2:B:88:ILE:HG22	2.11	0.50
2:B:27:ILE:HD12	2:B:27:ILE:N	2.26	0.50
1:A:569:GLN:C	1:A:571:GLN:H	2.15	0.49
2:B:82:MET:HE1	2:B:88:ILE:HD11	1.95	0.49
1:A:459:LYS:HZ2	2:B:69:GLN:NE2	2.10	0.49
2:B:29:GLN:HG3	2:B:91:TYR:HA	1.94	0.49
2:B:44:LEU:HD21	2:B:77:PRO:HD3	1.94	0.49
2:B:48:LYS:NZ	2:B:59:MET:SD	2.77	0.49
1:A:399:ARG:HH11	1:A:399:ARG:HG2	1.77	0.49
1:A:452:GLN:HG3	1:A:453:ALA:H	1.77	0.49
1:A:394:LYS:NZ	2:B:69:GLN:OE1	2.43	0.49
1:A:404:THR:HG21	1:A:412:ASN:OD1	2.12	0.49
1:A:459:LYS:NZ	2:B:69:GLN:NE2	2.60	0.49
2:B:59:MET:O	2:B:62:LEU:N	2.30	0.49
1:A:376:ILE:HG12	1:A:580:VAL:CG2	2.42	0.49
3:C:490:VAL:O	3:C:493:ALA:HB3	2.13	0.49
1:A:418:PHE:HD2	1:A:583:ILE:HG23	1.76	0.49
3:C:446:LEU:HA	3:C:449:LEU:HD12	1.95	0.49
1:A:470:LEU:HD13	1:A:556:ALA:HB1	1.94	0.49
3:C:573:SER:C	3:C:575:PHE:N	2.66	0.48
3:C:447:LEU:HD21	3:C:485:THR:HG22	1.94	0.48
2:B:74:ASN:N	2:B:74:ASN:HD22	2.11	0.48
1:A:580:VAL:O	1:A:584:LEU:HG	2.12	0.48
1:A:516:SER:O	1:A:518:THR:N	2.46	0.48
1:A:376:ILE:CG1	1:A:580:VAL:HG22	2.44	0.48
3:C:434:VAL:HG13	3:C:457:ILE:HD13	1.96	0.48
3:C:511:THR:O	3:C:512:PHE:C	2.52	0.48
2:B:53:GLN:HB3	2:B:54:ARG:HD3	1.95	0.48
3:C:523:LEU:O	3:C:524:LYS:HB2	2.13	0.48
1:A:376:ILE:CG1	1:A:580:VAL:CG2	2.92	0.48
1:A:393:PHE:HZ	1:A:422:LEU:HD23	1.79	0.48
1:A:516:SER:C	1:A:518:THR:H	2.16	0.48
1:A:544:ASN:C	1:A:544:ASN:ND2	2.62	0.47
3:C:448:ARG:HB2	3:C:448:ARG:NH1	2.29	0.47
3:C:437:PHE:CZ	3:C:446:LEU:HD13	2.49	0.47
1:A:484:ILE:CG2	1:A:491:LEU:HD23	2.42	0.47
1:A:511:TYR:CZ	1:A:515:GLU:HG3	2.49	0.47
1:A:530:THR:HG23	1:A:531:HIS:N	2.30	0.47
1:A:535:LYS:HB3	1:A:536:PRO:HD2	1.96	0.47
1:A:452:GLN:O	1:A:455:LYS:HG3	2.15	0.47
3:C:586:LYS:O	3:C:587:VAL:CG2	2.61	0.46
2:B:59:MET:C	2:B:61:SER:H	2.18	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:42:THR:HG22	2:B:43:HIS:N	2.30	0.46
1:A:376:ILE:HG22	1:A:377:SER:N	2.30	0.46
2:B:26:VAL:O	2:B:26:VAL:HG12	2.15	0.46
1:A:455:LYS:O	1:A:457:TRP:N	2.49	0.46
3:C:516:LEU:HG	3:C:520:MET:HE2	1.97	0.46
1:A:483:VAL:HG21	1:A:559:ILE:HG21	1.97	0.46
1:A:483:VAL:HG23	1:A:494:LEU:HD13	1.98	0.46
3:C:526:GLU:HG3	3:C:528:LYS:HG3	1.97	0.46
1:A:423:LEU:HD23	1:A:588:LEU:CD1	2.46	0.46
1:A:439:SER:O	1:A:442:PHE:HB3	2.16	0.46
1:A:585:HIS:O	1:A:586:GLN:HB2	2.16	0.46
1:A:494:LEU:HD12	1:A:494:LEU:N	2.31	0.45
3:C:552:PRO:O	3:C:554:ALA:N	2.49	0.45
2:B:27:ILE:CD1	2:B:27:ILE:H	2.28	0.45
3:C:555:LEU:O	3:C:556:ALA:C	2.55	0.45
2:B:40:MET:H	2:B:40:MET:HG2	1.39	0.45
2:B:65:LEU:HD23	2:B:68:GLY:O	2.16	0.45
3:C:534:ASN:O	3:C:538:PRO:HD2	2.16	0.45
1:A:402:ILE:HD11	1:A:580:VAL:HG23	1.99	0.45
3:C:580:LEU:O	3:C:580:LEU:HD23	2.17	0.45
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.72	0.45
3:C:443:PRO:HA	3:C:479:VAL:CG1	2.46	0.45
1:A:423:LEU:HD23	1:A:588:LEU:HD11	1.99	0.45
1:A:393:PHE:CZ	1:A:422:LEU:HD23	2.51	0.45
1:A:393:PHE:O	1:A:394:LYS:CB	2.64	0.45
2:B:34:ILE:O	2:B:34:ILE:HG22	2.17	0.44
1:A:490:CYS:HB2	1:A:530:THR:O	2.17	0.44
1:A:411:LEU:HG	1:A:549:GLY:HA3	1.99	0.44
3:C:447:LEU:CD2	3:C:485:THR:HG22	2.47	0.44
1:A:384:PRO:O	1:A:399:ARG:HG2	2.18	0.44
1:A:400:GLY:O	1:A:403:GLN:HB2	2.17	0.44
1:A:464:PHE:HD1	1:A:464:PHE:H	1.64	0.44
2:B:71:ILE:HG23	2:B:80:LEU:HD11	1.99	0.44
1:A:411:LEU:HD13	1:A:415:VAL:CG1	2.45	0.44
1:A:416:ILE:C	1:A:418:PHE:N	2.70	0.44
1:A:414:GLU:C	1:A:416:ILE:N	2.70	0.44
1:A:412:ASN:HA	2:B:95:THR:HG22	2.00	0.44
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.31	0.44
1:A:446:LEU:HD21	1:A:511:TYR:HB2	1.99	0.44
2:B:74:ASN:H	2:B:74:ASN:HD22	1.66	0.44
1:A:564:PRO:O	1:A:566:THR:HG23	2.18	0.44
2:B:51:TYR:C	2:B:53:GLN:H	2.20	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:36:PHE:C	2:B:37:LYS:HG3	2.37	0.43
1:A:484:ILE:HG23	1:A:491:LEU:CD2	2.45	0.43
1:A:570:HIS:C	1:A:571:GLN:HG3	2.39	0.43
3:C:524:LYS:O	3:C:525:SER:CB	2.66	0.43
3:C:556:ALA:N	3:C:557:PRO:CD	2.80	0.43
1:A:424:VAL:HG12	1:A:428:LYS:HE2	2.00	0.43
3:C:437:PHE:HA	3:C:445:LYS:HG2	2.01	0.43
3:C:437:PHE:HD1	3:C:445:LYS:CG	2.32	0.43
1:A:475:ARG:HH21	1:A:499:GLN:NE2	2.12	0.43
2:B:66:PHE:HD2	2:B:80:LEU:HD22	1.84	0.43
1:A:389:LEU:HD11	1:A:399:ARG:HD2	2.00	0.43
1:A:463:LEU:HG	1:A:469:ILE:CD1	2.45	0.43
1:A:455:LYS:C	1:A:457:TRP:H	2.21	0.43
1:A:563:LYS:HA	1:A:564:PRO:HD3	1.76	0.43
1:A:417:ASN:OD1	1:A:440:THR:HG23	2.19	0.43
1:A:475:ARG:O	1:A:476:LYS:C	2.58	0.43
1:A:491:LEU:HD11	1:A:509:LEU:HD13	2.00	0.43
1:A:525:ASN:O	1:A:529:TRP:CD1	2.67	0.43
3:C:448:ARG:CZ	3:C:448:ARG:HB2	2.49	0.43
2:B:23:LYS:HE2	2:B:37:LYS:NZ	2.34	0.42
1:A:554:LYS:HD3	1:A:554:LYS:HA	1.75	0.42
2:B:63:ARG:HD2	2:B:63:ARG:N	2.34	0.42
1:A:478:HIS:CE1	1:A:497:MET:HB2	2.54	0.42
1:A:499:GLN:HB2	3:C:515:ARG:CZ	2.49	0.42
3:C:515:ARG:HA	3:C:515:ARG:HD2	1.72	0.42
1:A:404:THR:HG21	1:A:412:ASN:CG	2.40	0.42
1:A:366:LEU:HB2	1:A:578:LYS:NZ	2.34	0.42
1:A:397:ILE:HD11	1:A:418:PHE:CG	2.54	0.42
1:A:517:LYS:HD2	1:A:523:ASP:OD1	2.18	0.42
1:A:434:ALA:HB3	1:A:467:GLU:H	1.83	0.42
1:A:393:PHE:HD1	1:A:418:PHE:CE1	2.37	0.42
2:B:59:MET:HA	2:B:62:LEU:HD12	2.01	0.42
1:A:411:LEU:N	1:A:411:LEU:CD2	2.82	0.42
1:A:544:ASN:ND2	1:A:547:ASP:H	2.15	0.42
1:A:365:LEU:HB3	1:A:366:LEU:H	1.69	0.42
3:C:438:LEU:O	3:C:439:ALA:C	2.57	0.42
2:B:44:LEU:CD2	2:B:77:PRO:HD3	2.50	0.42
3:C:448:ARG:CG	3:C:448:ARG:NH1	2.79	0.42
1:A:477:VAL:HG23	3:C:524:LYS:HD2	2.01	0.42
3:C:445:LYS:HB2	3:C:445:LYS:HZ2	1.84	0.42
1:A:477:VAL:HG21	3:C:524:LYS:HB3	2.02	0.42
3:C:477:SER:C	3:C:479:VAL:H	2.23	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:551:PHE:O	1:A:555:TYR:CG	2.73	0.42
2:B:30:ASP:O	2:B:31:SER:OG	2.34	0.42
1:A:376:ILE:HD11	1:A:577:LYS:O	2.20	0.41
3:C:523:LEU:HA	3:C:523:LEU:HD12	1.83	0.41
2:B:66:PHE:CD2	2:B:80:LEU:HD22	2.55	0.41
3:C:555:LEU:C	3:C:557:PRO:HD2	2.41	0.41
1:A:369:THR:HG21	1:A:372:MET:HG3	2.02	0.41
2:B:59:MET:O	2:B:61:SER:N	2.54	0.41
3:C:505:SER:O	3:C:507:PHE:N	2.54	0.41
3:C:545:MET:HG2	3:C:551:PHE:CD1	2.55	0.41
1:A:572:MET:N	1:A:573:PRO:CD	2.83	0.41
1:A:369:THR:HB	1:A:372:MET:HB2	2.02	0.41
3:C:453:SER:HA	3:C:456:LEU:HB2	2.03	0.41
1:A:410:TRP:CH2	1:A:477:VAL:HB	2.55	0.41
2:B:48:LYS:HE2	2:B:59:MET:HG3	2.02	0.41
1:A:433:PRO:HG2	1:A:487:ARG:HH12	1.85	0.41
1:A:416:ILE:C	1:A:418:PHE:H	2.25	0.41
1:A:574:LEU:O	1:A:575:PHE:C	2.59	0.41
3:C:488:MET:HA	3:C:491:GLN:HG3	2.02	0.41
2:B:40:MET:HA	2:B:77:PRO:CG	2.51	0.41
3:C:548:GLN:HA	3:C:548:GLN:NE2	2.36	0.41
1:A:496:SER:HB2	1:A:551:PHE:CD2	2.57	0.40
1:A:550:MET:HE1	1:A:579:MET:HG3	2.03	0.40
1:A:446:LEU:HD12	1:A:446:LEU:O	2.20	0.40
1:A:514:ASP:C	1:A:516:SER:H	2.24	0.40
1:A:585:HIS:C	1:A:586:GLN:HG3	2.41	0.40
1:A:517:LYS:HG2	1:A:517:LYS:O	2.22	0.40
3:C:461:THR:HG22	3:C:461:THR:O	2.20	0.40
1:A:438:PHE:HD2	1:A:438:PHE:HA	1.79	0.40
1:A:567:PHE:C	1:A:567:PHE:CD1	2.94	0.40
1:A:481:LEU:HD12	1:A:482:VAL:H	1.81	0.40
3:C:551:PHE:HA	3:C:552:PRO:HD2	1.93	0.40
1:A:572:MET:O	1:A:573:PRO:C	2.60	0.40
1:A:467:GLU:O	1:A:486:LEU:CB	2.69	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	Distance(Å)	Clash(Å)
4:A:2:HOH:O	4:A:2:HOH:O[7_555]	1.12	1.08

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	223/232 (96%)	170 (76%)	43 (19%)	10 (4%)	4	14
2	B	73/82 (89%)	50 (68%)	14 (19%)	9 (12%)	1	1
3	C	154/172 (90%)	110 (71%)	34 (22%)	10 (6%)	2	5
All	All	450/486 (93%)	330 (73%)	91 (20%)	29 (6%)	2	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	GLU
1	A	521	ASN
1	A	523	ASP
2	B	43	HIS
2	B	58	PRO
2	B	71	ILE
1	A	392	ALA
1	A	456	ARG
1	A	517	LYS
1	A	520	ARG
1	A	570	HIS
2	B	30	ASP
2	B	31	SER
2	B	32	SER
2	B	60	ASN
3	C	483	GLU
3	C	506	SER
3	C	553	LYS
1	A	455	LYS
2	B	41	THR
2	B	93	GLU
3	C	454	SER
3	C	484	ALA
3	C	487	ARG
3	C	514	THR

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Mol	Chain	Res	Type
3	C	525	SER
1	A	431	GLY
3	C	504	SER
3	C	552	PRO

5.3.2 Protein sidechains ⓘ

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	209/214 (98%)	182 (87%)	27 (13%)	6	17
2	B	68/73 (93%)	58 (85%)	10 (15%)	4	13
3	C	136/150 (91%)	120 (88%)	16 (12%)	8	22
All	All	413/437 (94%)	360 (87%)	53 (13%)	6	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	GLU
1	A	372	MET
1	A	386	ASP
1	A	398	THR
1	A	399	ARG
1	A	401	ASP
1	A	411	LEU
1	A	412	ASN
1	A	421	ASN
1	A	425	GLU
1	A	438	PHE
1	A	439	SER
1	A	447	LYS
1	A	475	ARG
1	A	476	LYS
1	A	486	LEU
1	A	490	CYS
1	A	491	LEU
1	A	492	LYS

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Mol	Chain	Res	Type
1	A	497	MET
1	A	530	THR
1	A	544	ASN
1	A	546	SER
1	A	548	SER
1	A	570	HIS
1	A	579	MET
1	A	580	VAL
2	B	36	PHE
2	B	38	VAL
2	B	40	MET
2	B	54	ARG
2	B	62	LEU
2	B	63	ARG
2	B	73	ASP
2	B	74	ASN
2	B	75	HIS
2	B	86	ASP
3	C	433	ASP
3	C	434	VAL
3	C	440	PHE
3	C	445	LYS
3	C	465	ASP
3	C	483	GLU
3	C	486	VAL
3	C	513	LEU
3	C	515	ARG
3	C	522	LEU
3	C	540	MET
3	C	549	ASP
3	C	558	LEU
3	C	562	PHE
3	C	574	SER
3	C	578	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	A	385	GLN
1	A	409	HIS
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	421	ASN
1	A	499	GLN
1	A	544	ASN
1	A	570	HIS
1	A	571	GLN
1	A	585	HIS
1	A	587	GLN
2	B	29	GLN
2	B	74	ASN
3	C	491	GLN
3	C	548	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	225/232 (96%)	0.29	14 (6%) 20 23	51, 88, 127, 159	0
2	B	75/82 (91%)	0.94	18 (24%) 1 2	57, 120, 143, 153	0
3	C	156/172 (90%)	-0.34	3 (1%) 64 72	36, 69, 117, 132	0
All	All	456/486 (93%)	0.18	35 (7%) 13 16	36, 87, 134, 159	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	7.1
2	B	23	LYS	6.5
1	A	417	ASN	4.4
1	A	528	GLU	4.1
1	A	439	SER	4.0
1	A	368	LEU	3.6
2	B	24	LEU	3.4
2	B	86	ASP	3.3
1	A	472	PRO	3.3
2	B	73	ASP	3.2
2	B	59	MET	3.1
2	B	69	GLN	3.1
2	B	82	MET	2.9
3	C	481	LYS	2.9
2	B	37	LYS	2.8
3	C	452	LYS	2.7
3	C	433	ASP	2.6
2	B	40	MET	2.6
1	A	471	VAL	2.6
1	A	463	LEU	2.5
2	B	56	GLY	2.5
2	B	68	GLY	2.4
2	B	34	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	380	LEU	2.4
1	A	553	CYS	2.3
2	B	79	GLU	2.2
1	A	384	PRO	2.2
2	B	29	GLN	2.2
1	A	416	ILE	2.2
2	B	43	HIS	2.1
1	A	578	LYS	2.1
2	B	49	GLU	2.1
1	A	420	MET	2.1
2	B	78	LYS	2.1
2	B	45	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.