



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 07:16 AM EDT

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 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 : 2.35
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) : 2.35

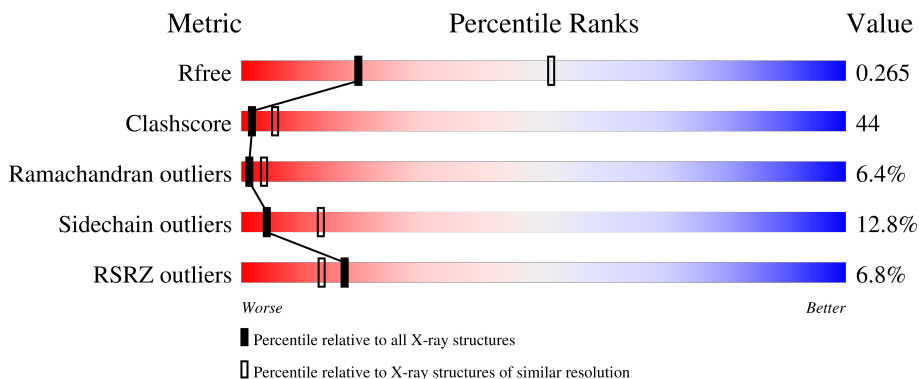
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	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 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 Sentrin-specific protease 2.

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

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 mutation	UNP Q9HC62

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

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

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
			Total	C	N	O	S			
3	C	156	1204	775	199	225	5	0	0	0

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 mutation	UNP P46060

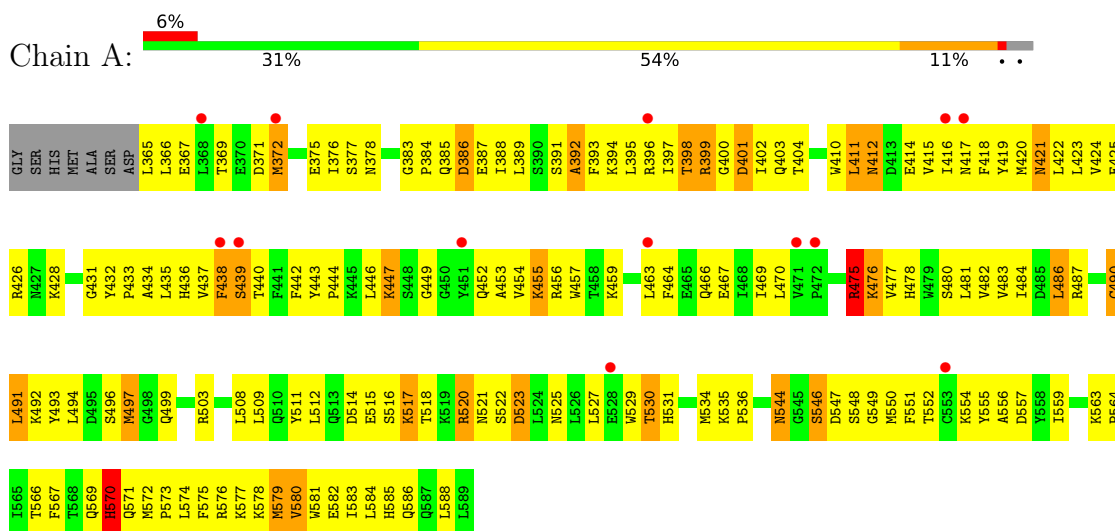
- Molecule 4 is water.

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

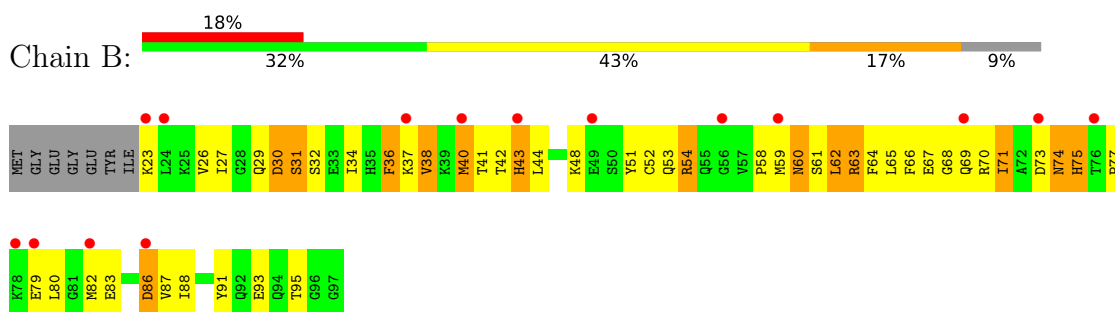
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

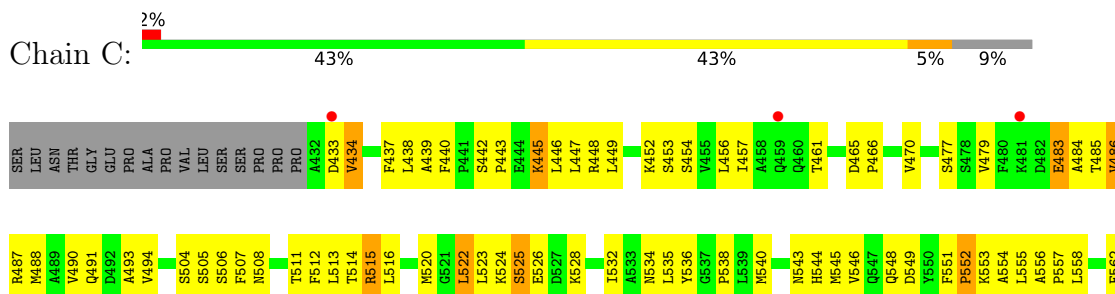
- Molecule 1: Sentrin-specific protease 2



- Molecule 2: Small ubiquitin-related modifier 1



- Molecule 3: Ran GTPase-activating protein 1



S572
S573
S574
F575
H578
S579
L580
L584
Y585
K586
V587

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	3.05 (at 2.90Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.301 0.261 , 0.265	Depositor DCC
R_{free} test set	678 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [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	0.39	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 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	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

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 44.

All (325) 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)
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
1:A:525:ASN:HD21	1:A:527:LEU:HB2	1.55	0.71
3:C:449:LEU:CB	3:C:453:SER:HB3	2.20	0.71
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:454:VAL:O	1:A:457:TRP:HB2	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:CG	1:A:477:VAL:HG13	2.24	0.68
3:C:434:VAL:CG1	3:C:457:ILE:HD13	2.24	0.68
1:A:573:PRO:O	1:A:576:ARG:HB2	1.93	0.68
3:C:552:PRO:HG2	3:C:555:LEU:HD12	1.75	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:27:ILE:HD12	2:B:27:ILE:H	1.60	0.66
2:B:82:MET:CE	2:B:88:ILE:HD11	2.26	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:HG3	3:C:448:ARG:HH11	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:366:LEU:HD13	1:A:578:LYS:NZ	2.14	0.62
1:A:525:ASN:O	1:A:529:TRP:HD1	1.82	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:HB2	3:C:445:LYS:NZ	2.15	0.62
1:A:412:ASN:HD21	1:A:415:VAL:H	1.48	0.61
1:A:411:LEU:N	1:A:411:LEU:HD23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:VAL:HA	1:A:435:LEU:HD23	1.82	0.61
1:A:393:PHE:O	1:A:394:LYS:HB2	2.00	0.60
1:A:412:ASN:ND2	1:A:415:VAL:H	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
1:A:436:HIS:HB3	1:A:469:ILE:HG12	1.83	0.59
1:A:443:TYR:HB3	1:A:444:PRO:HD3	1.84	0.59
1:A:499:GLN:NE2	3:C:515:ARG:NH2	2.50	0.59
2:B:36:PHE:O	2:B:37:LYS:CG	2.49	0.59
1:A:412:ASN:C	1:A:412:ASN:HD22	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:HD3	2:B:54:ARG:H	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
1:A:536:PRO:HB2	3:C:508:ASN:ND2	2.21	0.56
3:C:486:VAL:O	3:C:490:VAL:HG23	2.06	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:470:LEU:HD11	1:A:556:ALA:HB1	1.89	0.55
1:A:491:LEU:O	1:A:531:HIS:HA	2.06	0.55
1:A:520:ARG:C	1:A:522:SER:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:434:VAL:HG12	3:C:457:ILE:HD13	1.89	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
1:A:459:LYS:NZ	2:B:69:GLN:HE21	2.05	0.54
1:A:484:ILE:N	1:A:484:ILE:HD12	2.23	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:385:GLN:NE2	1:A:403:GLN:HG3	2.23	0.52
1:A:452:GLN:HG3	1:A:453:ALA:N	2.23	0.52
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:419:TYR:CD1	1:A:579:MET:SD	3.02	0.52
1:A:420:MET:O	1:A:437:VAL:HG21	2.09	0.52
1:A:512:LEU:O	1:A:515:GLU:N	2.42	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
2:B:64:PHE:CD1	2:B:64:PHE:N	2.79	0.51
3:C:488:MET:HA	3:C:491:GLN:HE21	1.75	0.51
2:B:79:GLU:O	2:B:79:GLU:HG2	2.11	0.51
3:C:528:LYS:O	3:C:532:ILE:HG13	2.11	0.51
1:A:483:VAL:HG11	1:A:559:ILE:CG2	2.40	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
3:C:452:LYS:O	3:C:456:LEU:HB2	2.11	0.51
1:A:366:LEU:HB2	1:A:578:LYS:HZ1	1.76	0.50
2:B:65:LEU:N	2:B:65:LEU:HD12	2.26	0.50
1:A:395:LEU:HD22	2:B:70:ARG:HD3	1.93	0.50
1:A:464:PHE:N	1:A:464:PHE:CD1	2.79	0.50
1:A:517:LYS:HB2	1:A:523:ASP:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ASN:HD22	1:A:546:SER:H	1.60	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
2:B:27:ILE:HD12	2:B:27:ILE:N	2.26	0.50
2:B:88:ILE:HG22	2:B:88:ILE:O	2.11	0.50
1:A:569:GLN:C	1:A:571:GLN:H	2.15	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:82:MET:HE1	2:B:88:ILE:HD11	1.95	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:394:LYS:NZ	2:B:69:GLN:OE1	2.43	0.49
1:A:452:GLN:HG3	1:A:453:ALA:H	1.77	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
1:A:418:PHE:HD2	1:A:583:ILE:HG23	1.76	0.49
3:C:490:VAL:O	3:C:493:ALA:HB3	2.13	0.49
1:A:470:LEU:HD13	1:A:556:ALA:HB1	1.94	0.49
3:C:446:LEU:HA	3:C:449:LEU:HD12	1.95	0.49
2:B:74:ASN:N	2:B:74:ASN:HD22	2.11	0.48
3:C:447:LEU:HD21	3:C:485:THR:HG22	1.94	0.48
3:C:573:SER:C	3:C:575:PHE:N	2.66	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
2:B:53:GLN:HB3	2:B:54:ARG:HD3	1.95	0.48
3:C:511:THR:O	3:C:512:PHE:C	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:42:THR:HG22	2:B:43:HIS:N	2.30	0.46
2:B:59:MET:C	2:B:61:SER:H	2.18	0.46
3:C:586:LYS:O	3:C:587:VAL:CG2	2.61	0.46
1:A:376:ILE:HG22	1:A:377:SER:N	2.30	0.46
2:B:26:VAL:HG12	2:B:26:VAL:O	2.15	0.46
1:A:455:LYS:O	1:A:457:TRP:N	2.49	0.46
1:A:483:VAL:HG21	1:A:559:ILE:HG21	1.97	0.46
3:C:516:LEU:HG	3:C:520:MET:HE2	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:N	1:A:494:LEU:HD12	2.31	0.45
2:B:27:ILE:H	2:B:27:ILE:CD1	2.28	0.45
3:C:552:PRO:O	3:C:554:ALA:N	2.49	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
1:A:508:LEU:HA	1:A:508:LEU:HD23	1.72	0.45
3:C:443:PRO:HA	3:C:479:VAL:CG1	2.46	0.45
3:C:580:LEU:O	3:C:580:LEU:HD23	2.17	0.45
1:A:423:LEU:HD23	1:A:588:LEU:HD11	1.99	0.45
1:A:393:PHE:O	1:A:394:LYS:CB	2.64	0.45
1:A:393:PHE:CZ	1:A:422:LEU:HD23	2.51	0.45
2:B:34:ILE:O	2:B:34:ILE:HG22	2.17	0.44
1:A:411:LEU:HG	1:A:549:GLY:HA3	1.99	0.44
1:A:490:CYS:HB2	1:A:530:THR:O	2.17	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: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:464:PHE:H	1:A:464:PHE:HD1	1.64	0.44
2:B:71:ILE:HG23	2:B:80:LEU:HD11	1.99	0.44
1:A:414:GLU:C	1:A:416:ILE:N	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.31	0.44
1:A:412:ASN:HA	2:B:95:THR:HG22	2.00	0.44
1:A:446:LEU:HD21	1:A:511:TYR:HB2	1.99	0.44
1:A:564:PRO:O	1:A:566:THR:HG23	2.18	0.44
2:B:74:ASN:HD22	2:B:74:ASN:H	1.66	0.44
2:B:51:TYR:C	2:B:53:GLN:H	2.20	0.44
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
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
3:C:437:PHE:HD1	3:C:445:LYS:CG	2.32	0.43
3:C:437:PHE:HA	3:C:445:LYS:HG2	2.01	0.43
1:A:389:LEU:HD11	1:A:399:ARG:HD2	2.00	0.43
1:A:417:ASN:OD1	1:A:440:THR:HG23	2.19	0.43
1:A:455:LYS:C	1:A:457:TRP:H	2.21	0.43
1:A:463:LEU:HG	1:A:469:ILE:CD1	2.45	0.43
1:A:563:LYS:HA	1:A:564:PRO:HD3	1.76	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:HB2	3:C:448:ARG:CZ	2.49	0.43
1:A:478:HIS:CE1	1:A:497:MET:HB2	2.54	0.42
1:A:554:LYS:HA	1:A:554:LYS:HD3	1.75	0.42
2:B:23:LYS:HE2	2:B:37:LYS:NZ	2.34	0.42
2:B:63:ARG:HD2	2:B:63:ARG:N	2.34	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:404:THR:HG21	1:A:412:ASN:CG	2.40	0.42
1:A:499:GLN:HB2	3:C:515:ARG:CZ	2.49	0.42
1:A:517:LYS:HD2	1:A:523:ASP:OD1	2.18	0.42
3:C:515:ARG:HD2	3:C:515:ARG:HA	1.72	0.42
1:A:393:PHE:HD1	1:A:418:PHE:CE1	2.37	0.42
1:A:434:ALA:HB3	1:A:467:GLU:H	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:477:VAL:HG21	3:C:524:LYS:HB3	2.02	0.42
3:C:445:LYS:HB2	3:C:445:LYS:HZ2	1.84	0.42
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
3:C:477:SER:C	3:C:479:VAL:H	2.23	0.42
1:A:376:ILE:HD11	1:A:577:LYS:O	2.20	0.41
2:B:66:PHE:CD2	2:B:80:LEU:HD22	2.55	0.41
3:C:523:LEU:HA	3:C:523:LEU:HD12	1.83	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
1:A:369:THR:HB	1:A:372:MET:HB2	2.02	0.41
1:A:572:MET:N	1:A:573:PRO:CD	2.83	0.41
3:C:545:MET:HG2	3:C:551:PHE:CD1	2.55	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
3:C:453:SER:HA	3:C:456:LEU:HB2	2.03	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
2:B:40:MET:HA	2:B:77:PRO:CG	2.51	0.41
3:C:488:MET:HA	3:C:491:GLN:HG3	2.02	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: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:550:MET:HE1	1:A:579:MET:HG3	2.03	0.40
1:A:585:HIS:C	1:A:586:GLN:HG3	2.41	0.40
1:A:438:PHE:HD2	1:A:438:PHE:HA	1.79	0.40
1:A:517:LYS:O	1:A:517:LYS:HG2	2.22	0.40
1:A:567:PHE:C	1:A:567:PHE:CD1	2.94	0.40
3:C:461:THR:O	3:C:461:THR:HG22	2.20	0.40
1:A:481:LEU:HD12	1:A:482:VAL:H	1.81	0.40
1:A:572:MET:O	1:A:573:PRO:C	2.60	0.40
3:C:551:PHE:HA	3:C:552:PRO:HD2	1.93	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	Interatomic distance (Å)	Clash overlap (Å)
4:A:2:HOH:O	4:A:2:HOH:O[7_555]	1.12	1.08

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	223/232 (96%)	170 (76%)	43 (19%)	10 (4%)	2	9
2	B	73/82 (89%)	50 (68%)	14 (19%)	9 (12%)	0	1
3	C	154/172 (90%)	110 (71%)	34 (22%)	10 (6%)	1	3
All	All	450/486 (93%)	330 (73%)	91 (20%)	29 (6%)	1	4

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

Continued on next page...

Continued from previous page...

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

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	209/214 (98%)	182 (87%)	27 (13%)	4 13
2	B	68/73 (93%)	58 (85%)	10 (15%)	3 9
3	C	136/150 (91%)	120 (88%)	16 (12%)	5 16
All	All	413/437 (94%)	360 (87%)	53 (13%)	4 13

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	574	SER
3	C	578	HIS

Sometimes 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
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 [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

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%)	0.33	13 (5%) 23 19	51, 88, 127, 159	0
2	B	75/82 (91%)	0.78	15 (20%) 1 0	57, 120, 143, 153	0
3	C	156/172 (90%)	-0.26	3 (1%) 66 65	36, 69, 117, 132	0
All	All	456/486 (93%)	0.20	31 (6%) 17 13	36, 87, 134, 159	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	6.3
2	B	23	LYS	6.1
1	A	439	SER	4.3
1	A	528	GLU	3.9
1	A	368	LEU	3.8
1	A	417	ASN	3.8
1	A	472	PRO	3.4
1	A	372	MET	3.2
2	B	59	MET	3.1
3	C	481	LYS	3.0
2	B	82	MET	2.9
1	A	553	CYS	2.9
3	C	433	ASP	2.9
2	B	40	MET	2.9
1	A	471	VAL	2.8
2	B	37	LYS	2.7
2	B	69	GLN	2.6
3	C	459	GLN	2.5
2	B	78	LYS	2.4
2	B	56	GLY	2.4
2	B	73	ASP	2.4
2	B	24	LEU	2.4
2	B	86	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	438	PHE	2.3
2	B	43	HIS	2.3
1	A	463	LEU	2.3
2	B	49	GLU	2.3
2	B	79	GLU	2.3
1	A	451	TYR	2.2
2	B	76	THR	2.2
1	A	416	ILE	2.1

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.