



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 PM UTC

PDB ID : 6XF1 / pdb_00006xf1
Title : Nesprin-2G(aa1425-1649)-FHOD1(aa1-339) complex, H. sapiens
Authors : Lim, S.M.; Schwartz, T.U.
Deposited on : 2020-06-15
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

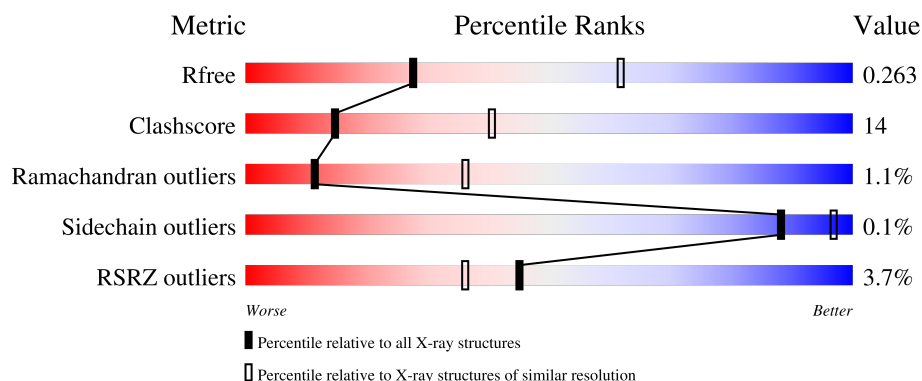
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	230	0% 82% 17% .
1	C	230	3% 67% 26% ...
2	B	321	6% 59% 32% ...
2	D	321	4% 67% 32% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8580 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 Nesprin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1892	1196	321	367	8			
1	C	224	Total	C	N	O	S	0	1	0
			1836	1162	311	355	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1420	PRO	-	expression tag	UNP Q8WXH0
A	1421	GLY	-	expression tag	UNP Q8WXH0
A	1422	SER	-	expression tag	UNP Q8WXH0
A	1423	GLU	-	expression tag	UNP Q8WXH0
A	1424	ASP	-	expression tag	UNP Q8WXH0
C	1420	PRO	-	expression tag	UNP Q8WXH0
C	1421	GLY	-	expression tag	UNP Q8WXH0
C	1422	SER	-	expression tag	UNP Q8WXH0
C	1423	GLU	-	expression tag	UNP Q8WXH0
C	1424	ASP	-	expression tag	UNP Q8WXH0

- Molecule 2 is a protein called FH1/FH2 domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2363	1509	390	455	9			
2	D	321	Total	C	N	O	S	0	0	0
			2465	1571	414	472	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

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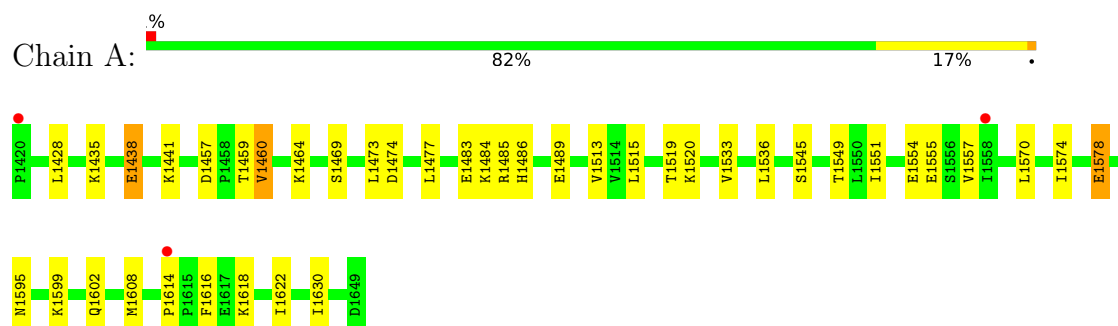
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	O 4	0	0
3	C	6	Total 6	O 6	0	0
3	D	7	Total 7	O 7	0	0

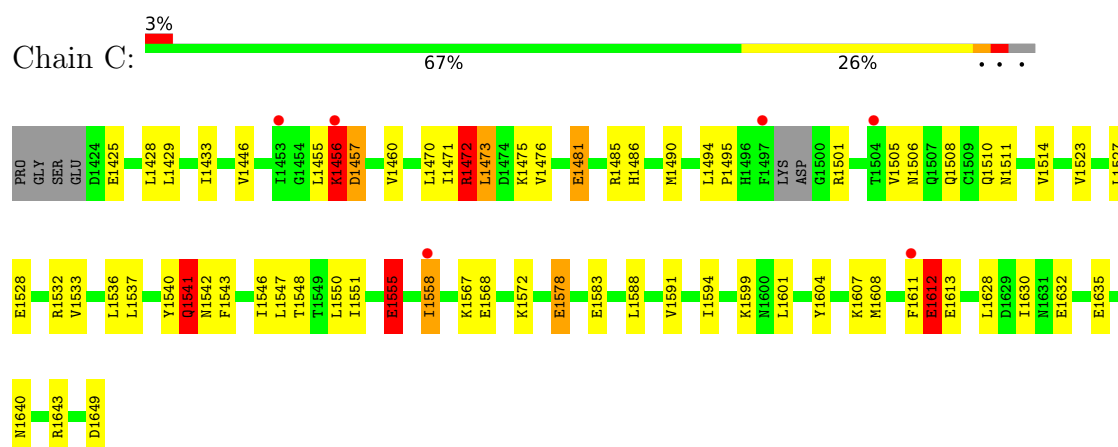
3 Residue-property plots [i](#)

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.

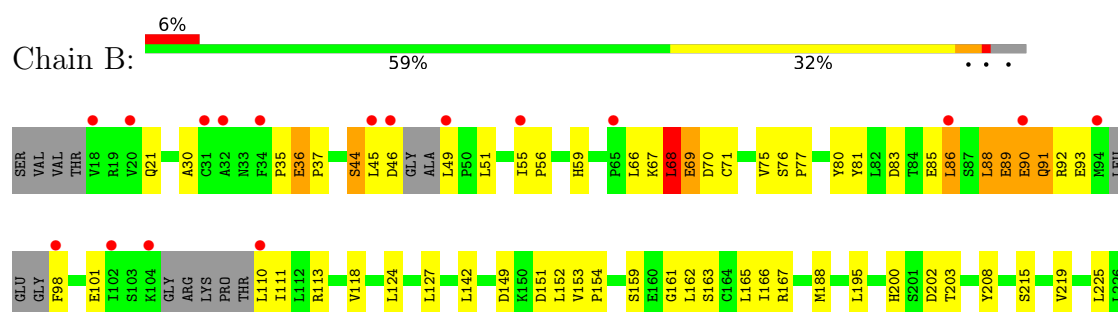
• Molecule 1: Nesprin-2

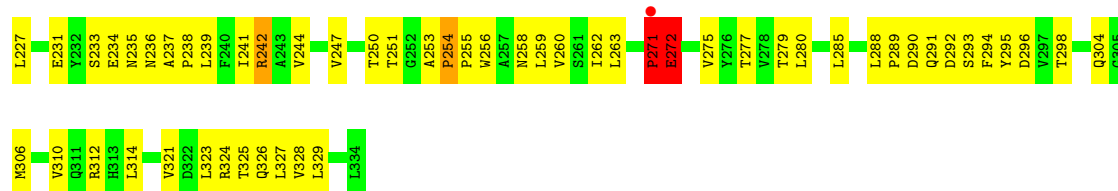


• Molecule 1: Nesprin-2

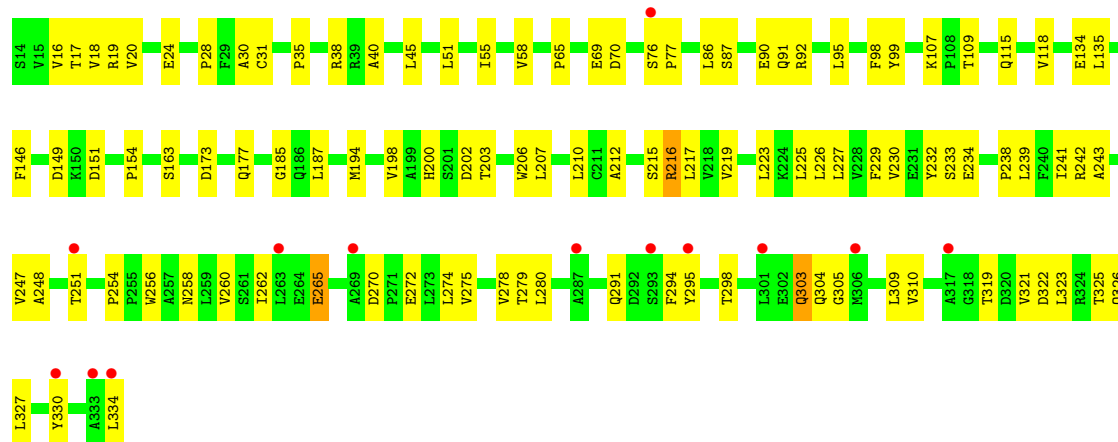


• Molecule 2: FH1/FH2 domain-containing protein 1





• Molecule 2: FH1/FH2 domain-containing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.82Å 52.44Å 177.46Å 90.00° 123.27° 90.00°	Depositor
Resolution (Å)	67.27 – 2.80 67.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (67.27-2.80) 98.6 (67.27-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.262 0.223 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8580	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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	0.68	2/1920 (0.1%)	0.94	9/2584 (0.3%)
1	C	0.77	3/1865 (0.2%)	1.41	28/2514 (1.1%)
2	B	0.56	1/2404 (0.0%)	1.03	15/3276 (0.5%)
2	D	0.52	2/2510 (0.1%)	0.89	9/3424 (0.3%)
All	All	0.63	8/8699 (0.1%)	1.07	61/11798 (0.5%)

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	1
1	C	0	5
2	B	0	4
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1460	VAL	CA-CB	-11.78	1.48	1.54
2	B	254	PRO	CA-C	-8.74	1.46	1.52
2	D	254	PRO	CA-C	-8.31	1.46	1.52
1	C	1473	LEU	N-CA	7.00	1.54	1.46
1	A	1485	ARG	CB-CG	-6.26	1.33	1.52
1	C	1460	VAL	CA-CB	5.91	1.57	1.54
1	C	1456	LYS	C-O	-5.83	1.16	1.24
2	D	35	PRO	C-N	5.69	1.49	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1612	GLU	CA-CB-CG	15.32	144.74	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1612	GLU	CB-CA-C	15.16	133.49	110.14
1	C	1555	GLU	CG-CD-OE1	13.80	150.15	118.40
1	C	1578	GLU	CG-CD-OE1	13.46	149.36	118.40
1	C	1578	GLU	OE1-CD-OE2	-13.08	91.51	122.90
1	A	1485	ARG	CG-CD-NE	-12.66	84.16	112.00
1	C	1555	GLU	OE1-CD-OE2	-12.30	93.38	122.90
1	C	1481	GLU	CB-CA-C	-11.45	91.84	110.84
1	C	1472	ARG	CG-CD-NE	-10.77	88.30	112.00
1	C	1555	GLU	CG-CD-OE2	-10.13	95.10	118.40
1	C	1578	GLU	CG-CD-OE2	-9.78	95.91	118.40
1	C	1472	ARG	NE-CZ-NH1	-9.48	112.02	121.50
2	B	86	LEU	CA-CB-CG	9.05	147.98	116.30
2	B	254	PRO	O-C-N	-9.02	116.91	121.15
2	D	254	PRO	O-C-N	-8.63	117.09	121.15
1	C	1472	ARG	CD-NE-CZ	8.49	136.28	124.40
2	D	134	GLU	CA-CB-CG	8.38	130.85	114.10
1	C	1455	LEU	CA-C-N	8.02	136.86	121.54
1	C	1455	LEU	C-N-CA	8.02	136.86	121.54
2	B	272	GLU	CA-CB-CG	7.40	128.90	114.10
1	C	1541	GLN	CA-CB-CG	7.40	128.90	114.10
1	C	1475	LYS	CG-CD-CE	7.39	128.29	111.30
2	B	36	GLU	CA-CB-CG	-7.03	100.04	114.10
1	A	1485	ARG	CB-CG-CD	6.93	127.23	111.30
1	C	1475	LYS	CA-CB-CG	6.75	127.61	114.10
2	B	44	SER	CA-C-N	-6.73	108.69	121.54
2	B	44	SER	C-N-CA	-6.73	108.69	121.54
1	C	1471	ILE	CA-C-N	-6.65	110.71	120.28
1	C	1471	ILE	C-N-CA	-6.65	110.71	120.28
1	C	1425	GLU	CA-CB-CG	6.61	127.32	114.10
2	D	18	VAL	CA-C-N	6.45	132.08	123.05
2	D	18	VAL	C-N-CA	6.45	132.08	123.05
1	C	1612	GLU	CA-C-N	6.43	137.50	121.80
1	C	1612	GLU	C-N-CA	6.43	137.50	121.80
2	D	216	ARG	CB-CA-C	6.17	123.21	110.31
1	C	1541	GLN	CB-CA-C	-5.87	98.74	110.42
1	A	1428	LEU	CA-CB-CG	5.84	136.75	116.30
2	B	89	GLU	CA-CB-CG	-5.84	102.42	114.10
2	D	303	GLN	CA-CB-CG	-5.82	102.46	114.10
2	B	291	GLN	CA-C-N	5.79	130.39	120.71
2	B	291	GLN	C-N-CA	5.79	130.39	120.71
1	C	1475	LYS	CB-CA-C	-5.63	101.44	110.79
2	B	271	PRO	CA-C-N	5.60	132.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	271	PRO	C-N-CA	5.60	132.23	121.54
2	D	134	GLU	CB-CA-C	-5.59	102.03	110.92
1	A	1578	GLU	CB-CG-CD	5.59	122.09	112.60
2	B	88	LEU	CA-C-N	-5.57	111.21	120.68
2	B	88	LEU	C-N-CA	-5.57	111.21	120.68
2	B	272	GLU	N-CA-CB	-5.48	101.22	110.49
1	A	1578	GLU	CA-C-N	-5.47	112.96	120.46
1	A	1578	GLU	C-N-CA	-5.47	112.96	120.46
1	C	1611	PHE	CA-C-N	-5.40	114.40	122.39
1	C	1611	PHE	C-N-CA	-5.40	114.40	122.39
1	A	1578	GLU	CA-CB-CG	5.38	124.85	114.10
2	D	216	ARG	N-CA-CB	-5.24	101.69	110.39
2	B	242	ARG	CB-CG-CD	-5.21	99.31	111.30
1	C	1472	ARG	N-CA-CB	5.18	118.20	110.22
1	A	1438	GLU	CA-CB-CG	5.15	124.40	114.10
2	D	134	GLU	N-CA-CB	5.08	117.53	109.82
1	A	1485	ARG	CB-CA-C	5.05	119.43	110.85
1	C	1578	GLU	CB-CA-C	5.04	119.15	110.79

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1578	GLU	Sidechain
2	B	271	PRO	Peptide
2	B	272	GLU	Sidechain
2	B	68	LEU	Peptide
2	B	90	GLU	Peptide
1	C	1472	ARG	Sidechain
1	C	1555	GLU	Sidechain
1	C	1558	ILE	Peptide
1	C	1578	GLU	Sidechain
1	C	1612	GLU	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	1892	0	1906	24	0
1	C	1836	0	1834	45	0
2	B	2363	0	2347	94	0
2	D	2465	0	2469	78	0
3	A	7	0	0	0	0
3	B	4	0	0	1	0
3	C	6	0	0	0	0
3	D	7	0	0	0	0
All	All	8580	0	8556	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (237) 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:236:ASN:HA	2:B:239:LEU:HD23	1.50	0.91
2:B:75:VAL:HA	2:B:110:LEU:HD13	1.56	0.87
1:C:1532:ARG:NH2	1:C:1604:TYR:OH	2.08	0.86
1:C:1528:GLU:OE2	2:D:38:ARG:NH1	2.09	0.85
1:A:1602:GLN:OE1	1:A:1616:PHE:N	2.10	0.84
2:B:166:ILE:HD11	2:B:203:THR:HA	1.59	0.83
2:D:69:GLU:N	2:D:69:GLU:OE1	2.12	0.82
2:D:216:ARG:NH2	2:D:270:ASP:OD1	2.12	0.82
1:C:1470:LEU:HB3	1:C:1527:LEU:HD11	1.61	0.82
2:B:323:LEU:O	2:B:327:LEU:HD12	1.82	0.80
2:D:310:VAL:HG13	2:D:327:LEU:HD11	1.66	0.76
2:B:290:ASP:OD2	2:B:293:SER:N	2.17	0.75
2:D:24:GLU:OE1	2:D:65:PRO:HG2	1.87	0.74
1:A:1477:LEU:HD11	1:A:1519:THR:HG22	1.71	0.73
1:C:1640:ASN:OD1	1:C:1643:ARG:NH2	2.22	0.72
2:B:55:ILE:HG13	2:B:56:PRO:HD3	1.71	0.72
2:D:325:THR:OG1	2:D:326:GLN:OE1	2.06	0.72
2:B:88:LEU:HD13	2:B:91:GLN:OE1	1.90	0.70
2:B:70:ASP:HB3	2:B:118:VAL:HG21	1.74	0.70
1:A:1438:GLU:OE1	1:A:1441:LYS:NZ	2.25	0.69
1:A:1618:LYS:O	1:A:1622:ILE:HG12	1.93	0.69
2:B:238:PRO:HA	2:B:241:ILE:HG12	1.75	0.68
2:B:127:LEU:HD21	2:B:142:LEU:HD11	1.75	0.68
2:B:290:ASP:HB3	2:B:293:SER:HB2	1.74	0.68
1:A:1551:ILE:O	1:A:1555:GLU:HB2	1.95	0.67
1:C:1429:LEU:O	1:C:1433:ILE:HG12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:MET:O	2:D:198:VAL:HG23	1.95	0.67
2:B:81:TYR:OH	2:B:113:ARG:NH1	2.28	0.66
1:C:1567:LYS:NZ	1:C:1649:ASP:OD2	2.27	0.66
1:A:1551:ILE:HG12	1:A:1630:ILE:HG21	1.78	0.66
2:D:326:GLN:OE1	2:D:326:GLN:N	2.29	0.65
2:B:306:MET:O	2:B:310:VAL:HG23	1.96	0.65
2:D:19:ARG:HB2	2:D:109:THR:HG22	1.79	0.65
2:D:206:TRP:O	2:D:210:LEU:HD23	1.97	0.65
1:C:1540:TYR:O	1:C:1541:GLN:C	2.40	0.64
2:B:275:VAL:O	2:B:279:THR:HG23	1.98	0.64
2:D:270:ASP:C	2:D:274:LEU:HD22	2.22	0.64
2:B:288:LEU:HD12	2:B:289:PRO:HD2	1.81	0.63
2:B:44:SER:O	2:B:45:LEU:HD12	1.99	0.62
2:D:19:ARG:CB	2:D:109:THR:HG22	2.30	0.62
1:C:1542:ASN:O	1:C:1546:ILE:HG13	1.98	0.62
2:B:279:THR:HG22	2:B:326:GLN:CD	2.24	0.61
2:B:312:ARG:HH11	2:B:312:ARG:HG2	1.65	0.61
2:B:86:LEU:CB	2:B:89:GLU:H	2.13	0.61
2:B:256:TRP:HE3	2:B:259:LEU:HD12	1.66	0.61
2:B:83:ASP:N	2:B:90:GLU:OE2	2.33	0.61
2:B:149:ASP:HB3	2:B:152:LEU:HD12	1.83	0.61
2:D:203:THR:O	2:D:207:LEU:HD12	2.01	0.60
2:B:227:LEU:HD21	2:B:280:LEU:HA	1.84	0.60
2:B:49:LEU:HD13	2:B:88:LEU:HD23	1.84	0.60
2:D:272:GLU:H	2:D:272:GLU:CD	2.09	0.59
2:D:194:MET:HE1	2:D:229:PHE:HA	1.85	0.59
1:A:1545:SER:O	1:A:1549:THR:HG23	2.03	0.59
1:C:1588:LEU:O	1:C:1591:VAL:HG12	2.03	0.59
2:D:322:ASP:O	2:D:326:GLN:OE1	2.20	0.58
2:B:59:HIS:NE2	2:B:66:LEU:O	2.37	0.58
1:C:1555:GLU:HG3	1:C:1630:ILE:HD13	1.84	0.58
2:D:16:VAL:HG23	2:D:45:LEU:HB2	1.85	0.58
2:D:275:VAL:O	2:D:279:THR:HG23	2.04	0.58
2:B:86:LEU:HB3	2:B:89:GLU:H	1.69	0.58
2:D:241:ILE:HG23	2:D:256:TRP:HZ2	1.69	0.58
2:B:241:ILE:O	2:B:244:VAL:HG22	2.04	0.57
2:D:265:GLU:O	2:D:265:GLU:HG2	2.04	0.57
2:B:166:ILE:HD11	2:B:203:THR:CA	2.29	0.57
2:B:260:VAL:HG12	2:B:263:LEU:HD12	1.85	0.57
1:C:1428:LEU:HD21	1:C:1495:PRO:HD3	1.85	0.57
1:C:1635:GLU:HG2	2:D:217:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:MET:CE	2:B:225:LEU:HD22	2.35	0.57
1:C:1551:ILE:O	1:C:1555:GLU:HB2	2.05	0.57
2:B:295:TYR:HA	2:B:298:THR:HG22	1.87	0.56
2:D:260:VAL:HG21	2:D:304:GLN:HG2	1.86	0.56
2:B:188:MET:HE1	2:B:225:LEU:HD22	1.87	0.56
2:B:260:VAL:HA	2:B:263:LEU:HD12	1.88	0.56
1:C:1548:THR:HA	1:C:1551:ILE:HG12	1.87	0.56
2:D:212:ALA:HB2	2:D:258:ASN:OD1	2.05	0.56
2:B:285:LEU:HD22	2:B:294:PHE:CD1	2.42	0.55
2:D:270:ASP:O	2:D:274:LEU:HD22	2.07	0.55
2:B:208:TYR:CD1	2:B:247:VAL:HG11	2.42	0.55
2:D:238:PRO:O	2:D:242:ARG:HG3	2.07	0.55
1:A:1457:ASP:HB2	1:A:1459:THR:HG23	1.88	0.55
2:B:75:VAL:HA	2:B:110:LEU:CD1	2.33	0.55
2:B:256:TRP:CE3	2:B:259:LEU:HD12	2.41	0.54
2:B:76:SER:HB3	2:B:77:PRO:HD3	1.88	0.54
1:C:1506:ASN:O	1:C:1510:GLN:HG2	2.06	0.54
2:B:89:GLU:O	2:B:89:GLU:HG3	2.07	0.54
1:C:1428:LEU:HD11	1:C:1494:LEU:HB2	1.88	0.54
2:D:95:LEU:HB3	2:D:98:PHE:HB3	1.89	0.53
2:B:326:GLN:HA	2:B:329:LEU:HD13	1.90	0.53
1:A:1554:GLU:O	1:A:1557:VAL:HG12	2.08	0.53
2:D:146:PHE:CE2	2:D:187:LEU:HD11	2.43	0.53
2:D:19:ARG:HD3	2:D:40:ALA:HB3	1.91	0.53
2:D:243:ALA:O	2:D:247:VAL:HG23	2.08	0.53
2:D:86:LEU:HB2	2:D:90:GLU:OE1	2.08	0.52
1:A:1484:LYS:HG2	1:A:1513:VAL:HG22	1.91	0.52
1:C:1537:LEU:HD23	1:C:1601:LEU:HD11	1.91	0.52
1:A:1469:SER:O	1:A:1473:LEU:HD22	2.11	0.51
2:D:272:GLU:OE1	2:D:272:GLU:N	2.33	0.51
2:B:91:GLN:HG2	2:B:92:ARG:N	2.26	0.51
2:B:254:PRO:HB2	2:B:304:GLN:NE2	2.25	0.51
2:D:70:ASP:HB3	2:D:118:VAL:HG21	1.91	0.51
2:D:206:TRP:CE2	2:D:210:LEU:HD21	2.45	0.51
1:A:1602:GLN:HE22	1:A:1614:PRO:HB3	1.76	0.51
2:D:92:ARG:HG3	2:D:99:TYR:CE2	2.46	0.51
2:D:216:ARG:HH21	2:D:270:ASP:CG	2.12	0.51
2:B:237:ALA:HB3	2:B:238:PRO:HD3	1.93	0.50
1:C:1446:VAL:HG23	1:C:1473:LEU:HD22	1.93	0.50
2:B:247:VAL:HA	2:B:250:THR:HG22	1.92	0.50
1:C:1568:GLU:O	1:C:1572:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:VAL:HG12	2:B:80:TYR:O	2.12	0.50
2:B:256:TRP:O	2:B:260:VAL:HG22	2.12	0.50
1:C:1508:GLN:O	1:C:1511:ASN:HB2	2.11	0.50
2:D:321:VAL:O	2:D:325:THR:HG23	2.12	0.50
1:C:1523:VAL:O	1:C:1527:LEU:HD13	2.12	0.49
2:B:324:ARG:HA	2:B:327:LEU:HD13	1.94	0.49
2:B:83:ASP:O	2:B:85:GLU:N	2.45	0.49
2:D:185:GLY:HA2	2:D:225:LEU:HD11	1.94	0.49
2:B:151:ASP:N	2:B:151:ASP:OD1	2.46	0.49
2:D:215:SER:O	2:D:219:VAL:HG23	2.12	0.49
2:B:21:GLN:O	2:B:111:ILE:HA	2.13	0.49
2:B:251:THR:HG23	2:B:253:ALA:H	1.78	0.49
1:C:1533:VAL:HG21	1:C:1608:MET:HE3	1.94	0.48
2:D:233:SER:OG	2:D:234:GLU:N	2.46	0.48
2:D:303:GLN:O	2:D:303:GLN:HG2	2.13	0.48
1:C:1473:LEU:O	1:C:1476:VAL:HG22	2.13	0.48
1:C:1472:ARG:HG3	1:C:1473:LEU:N	2.28	0.48
2:B:238:PRO:O	2:B:242:ARG:HG3	2.14	0.48
2:B:321:VAL:O	2:B:325:THR:OG1	2.24	0.48
1:A:1474:ASP:OD2	1:A:1520:LYS:HE2	2.14	0.48
1:C:1433:ILE:HD11	1:C:1505:VAL:HG11	1.95	0.48
2:D:70:ASP:O	2:D:115:GLN:HG3	2.14	0.48
2:D:226:LEU:O	2:D:230:VAL:HG12	2.14	0.48
2:D:86:LEU:HD12	2:D:90:GLU:HB3	1.95	0.48
1:C:1550:LEU:HD11	1:C:1583:GLU:HG2	1.95	0.47
2:B:88:LEU:O	2:B:91:GLN:HB3	2.14	0.47
2:B:68:LEU:O	2:B:71:CYS:HB2	2.15	0.47
2:B:275:VAL:HG22	2:B:323:LEU:HB2	1.97	0.47
2:D:76:SER:HB3	2:D:77:PRO:HD3	1.96	0.47
2:B:153:VAL:HG22	2:B:154:PRO:HD3	1.97	0.46
2:B:325:THR:O	2:B:328:VAL:HG22	2.16	0.46
2:B:21:GLN:NE2	2:B:37:PRO:O	2.33	0.46
1:A:1438:GLU:OE1	1:A:1441:LYS:CE	2.64	0.46
1:C:1486:HIS:O	1:C:1490:MET:HG3	2.16	0.46
2:B:124:LEU:HD21	2:B:161:GLY:HA2	1.97	0.45
1:C:1604:TYR:O	1:C:1608:MET:HG3	2.16	0.45
2:D:17:THR:HG22	2:D:107:LYS:HG2	1.99	0.45
2:D:227:LEU:HA	2:D:227:LEU:HD23	1.67	0.45
2:D:20:VAL:HG21	2:D:58:VAL:HG23	1.98	0.45
1:C:1456:LYS:O	1:C:1457:ASP:HB2	2.15	0.45
2:D:226:LEU:HD23	2:D:226:LEU:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:PRO:C	2:B:36:GLU:HG2	2.40	0.45
2:B:200:HIS:CE1	2:B:202:ASP:HB2	2.52	0.44
2:B:233:SER:OG	2:B:234:GLU:N	2.49	0.44
2:B:86:LEU:HD12	2:B:88:LEU:HB2	1.99	0.44
2:D:275:VAL:HA	2:D:278:VAL:HG12	1.99	0.44
2:D:305:GLY:O	2:D:309:LEU:HD13	2.17	0.44
2:B:215:SER:O	2:B:219:VAL:HG23	2.17	0.44
2:B:227:LEU:O	2:B:231:GLU:HG3	2.17	0.44
2:B:290:ASP:OD2	2:B:292:ASP:HB3	2.17	0.44
2:B:188:MET:HE3	2:B:188:MET:HB2	1.73	0.44
2:D:279:THR:HG22	2:D:326:GLN:HG2	1.99	0.44
1:C:1470:LEU:HB3	1:C:1527:LEU:CD1	2.40	0.44
2:D:163:SER:CA	2:D:200:HIS:HE1	2.30	0.44
1:A:1460:VAL:O	1:A:1464:LYS:HG2	2.18	0.43
1:A:1533:VAL:HG21	1:A:1608:MET:HE3	2.00	0.43
1:A:1435:LYS:NZ	1:A:1483:GLU:OE2	2.50	0.43
1:C:1533:VAL:HG21	1:C:1608:MET:CE	2.48	0.43
2:B:242:ARG:HH21	2:B:242:ARG:HD2	1.67	0.43
2:B:244:VAL:HG21	2:B:256:TRP:CZ2	2.53	0.43
2:B:195:LEU:HD23	2:B:195:LEU:HA	1.81	0.43
2:D:135:LEU:HD12	2:D:135:LEU:HA	1.74	0.43
2:D:173:ASP:O	2:D:177:GLN:HG3	2.17	0.43
2:B:271:PRO:O	2:B:275:VAL:HG23	2.19	0.43
1:A:1536:LEU:HA	1:A:1536:LEU:HD23	1.81	0.43
1:C:1536:LEU:HA	1:C:1536:LEU:HD23	1.77	0.43
1:C:1543:PHE:CB	1:C:1594:ILE:HD12	2.49	0.43
2:B:70:ASP:CB	2:B:118:VAL:HG21	2.48	0.43
2:B:258:ASN:O	2:B:262:ILE:HG12	2.19	0.43
2:D:200:HIS:NE2	2:D:202:ASP:HB2	2.34	0.43
2:B:235:ASN:O	2:B:238:PRO:HD2	2.19	0.42
2:D:258:ASN:O	2:D:262:ILE:HG13	2.19	0.42
2:D:227:LEU:HD21	2:D:280:LEU:HA	2.00	0.42
2:B:255:PRO:O	2:B:304:GLN:NE2	2.52	0.42
2:D:219:VAL:O	2:D:223:LEU:HD23	2.18	0.42
2:D:330:TYR:C	2:D:330:TYR:CD2	2.96	0.42
1:A:1595:ASN:O	1:A:1599:LYS:HG3	2.20	0.42
2:B:51:LEU:HD23	2:B:51:LEU:HA	1.66	0.42
2:B:312:ARG:HG2	2:B:312:ARG:NH1	2.33	0.42
1:C:1628:LEU:O	1:C:1632:GLU:HG3	2.20	0.42
2:D:227:LEU:HA	2:D:230:VAL:HG12	2.02	0.42
1:C:1599:LYS:HG2	2:D:30:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LEU:HD22	2:B:277:THR:HG23	2.02	0.42
1:C:1501:ARG:O	1:C:1505:VAL:HG22	2.20	0.42
1:C:1506:ASN:OD1	1:C:1506:ASN:C	2.62	0.42
2:D:200:HIS:CD2	2:D:202:ASP:HB2	2.55	0.42
2:D:294:PHE:HE2	2:D:334:LEU:HD21	1.85	0.42
2:B:124:LEU:HD11	2:B:159:SER:O	2.20	0.42
2:B:324:ARG:HA	2:B:327:LEU:CD1	2.50	0.42
1:C:1428:LEU:HD11	1:C:1495:PRO:CD	2.50	0.42
1:C:1481:GLU:OE1	1:C:1485:ARG:NH1	2.53	0.42
2:B:293:SER:O	2:B:296:ASP:HB3	2.20	0.42
2:D:194:MET:HG2	2:D:232:TYR:CE1	2.55	0.41
2:D:194:MET:HG2	2:D:232:TYR:CD1	2.55	0.41
2:D:239:LEU:CD1	2:D:242:ARG:HH11	2.34	0.41
2:D:291:GLN:O	2:D:294:PHE:HB3	2.21	0.41
2:B:67:LYS:CB	2:B:69:GLU:OE1	2.69	0.41
2:D:87:SER:O	2:D:91:GLN:HG2	2.21	0.41
1:A:1486:HIS:O	1:A:1489:GLU:HB3	2.21	0.41
2:B:46:ASP:O	2:B:49:LEU:HD23	2.21	0.41
2:B:310:VAL:HG12	2:B:314:LEU:HD11	2.02	0.41
1:C:1510:GLN:O	1:C:1514:VAL:HG23	2.21	0.41
1:A:1438:GLU:OE1	1:A:1441:LYS:HE3	2.19	0.41
2:B:255:PRO:HB2	2:B:256:TRP:CD1	2.55	0.41
2:D:149:ASP:OD2	2:D:151:ASP:HB2	2.20	0.41
2:B:81:TYR:HE1	2:B:151:ASP:OD2	2.04	0.41
2:D:51:LEU:O	2:D:55:ILE:HG13	2.20	0.41
1:A:1570:LEU:O	1:A:1574:ILE:HG13	2.21	0.41
2:B:162:LEU:HD23	2:B:162:LEU:HA	1.86	0.41
1:C:1547:LEU:HD23	1:C:1547:LEU:HA	1.87	0.41
2:D:28:PRO:HA	2:D:31:CYS:SG	2.60	0.41
1:C:1548:THR:HA	1:C:1551:ILE:CG1	2.51	0.41
1:A:1515:LEU:HD12	1:A:1515:LEU:HA	1.87	0.40
2:B:163:SER:O	2:B:167:ARG:HB3	2.21	0.40
1:C:1537:LEU:HD23	1:C:1537:LEU:HA	1.72	0.40
2:D:151:ASP:O	2:D:154:PRO:HD2	2.21	0.40
2:D:294:PHE:CE2	2:D:334:LEU:HD21	2.55	0.40
2:D:319:THR:HG23	2:D:323:LEU:HD23	2.02	0.40
1:A:1599:LYS:HD3	2:B:30:ALA:HA	2.02	0.40
2:B:98:PHE:O	2:B:101:GLU:OE1	2.40	0.40
2:B:110:LEU:N	3:B:401:HOH:O	2.54	0.40
2:B:165:LEU:HD23	2:B:165:LEU:HA	1.84	0.40
2:D:248:ALA:HA	2:D:251:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:PHE:CD2	2:D:294:PHE:C	2.99	0.40
1:C:1456:LYS:N	1:C:1456:LYS:HD2	2.37	0.40
1:C:1607:LYS:HE3	1:C:1607:LYS:HB3	1.78	0.40
2:D:163:SER:HA	2:D:200:HIS:HE1	1.86	0.40
2:B:208:TYR:HD1	2:B:247:VAL:HG11	1.85	0.40
2:D:295:TYR:HA	2:D:298:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/230 (99%)	227 (100%)	1 (0%)	0	100	100
1	C	221/230 (96%)	213 (96%)	2 (1%)	6 (3%)	4	15
2	B	299/321 (93%)	281 (94%)	13 (4%)	5 (2%)	7	25
2	D	319/321 (99%)	309 (97%)	9 (3%)	1 (0%)	36	66
All	All	1067/1102 (97%)	1030 (96%)	25 (2%)	12 (1%)	11	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	GLU
2	D	265	GLU
2	B	68	LEU
2	B	69	GLU
2	B	91	GLN
2	B	93	GLU
1	C	1456	LYS
1	C	1541	GLN
1	C	1555	GLU

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Mol	Chain	Res	Type
1	C	1613	GLU
1	C	1457	ASP
1	C	1558	ILE

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	214/215 (100%)	214 (100%)	0	100	100
1	C	206/215 (96%)	205 (100%)	1 (0%)	81	93
2	B	258/276 (94%)	258 (100%)	0	100	100
2	D	269/276 (98%)	269 (100%)	0	100	100
All	All	947/982 (96%)	946 (100%)	1 (0%)	88	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1612	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1596	GLN
2	B	158	HIS
2	D	177	GLN
2	D	304	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 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	230/230 (100%)	0.04	3 (1%) 75 66	48, 66, 109, 147	0
1	C	224/230 (97%)	0.45	6 (2%) 56 46	70, 92, 146, 177	1 (0%)
2	B	307/321 (95%)	0.55	18 (5%) 28 21	54, 103, 171, 205	0
2	D	321/321 (100%)	0.42	13 (4%) 42 33	54, 98, 183, 232	0
All	All	1082/1102 (98%)	0.38	40 (3%) 45 36	48, 91, 170, 232	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	VAL	4.9
2	D	334	LEU	4.1
2	B	49	LEU	4.1
1	C	1504	THR	3.6
2	D	269	ALA	3.5
2	B	98	PHE	3.4
2	B	45	LEU	3.3
1	C	1558	ILE	3.3
2	B	46	ASP	3.2
2	B	90	GLU	3.1
1	A	1420	PRO	3.1
2	D	76	SER	3.0
1	C	1611	PHE	2.9
2	B	102	ILE	2.9
2	B	31	CYS	2.9
2	B	34	PHE	2.8
2	D	287	ALA	2.8
1	C	1453	ILE	2.8
2	B	271	PRO	2.7
2	B	104	LYS	2.7
2	B	32	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	65	PRO	2.6
2	D	317	ALA	2.5
2	B	86	LEU	2.5
2	D	306	MET	2.5
1	C	1497	PHE	2.4
2	D	251	THR	2.4
2	B	94	MET	2.4
2	D	333	ALA	2.3
1	C	1456	LYS	2.3
2	B	55	ILE	2.3
2	D	293	SER	2.2
2	B	110	LEU	2.2
2	D	295	TYR	2.2
2	B	20	VAL	2.2
2	D	301	LEU	2.2
1	A	1614	PRO	2.1
2	D	330	TYR	2.1
1	A	1558	ILE	2.0
2	D	263	LEU	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.