Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 11:16 PM EDT

PDB ID	:	6XF1
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:

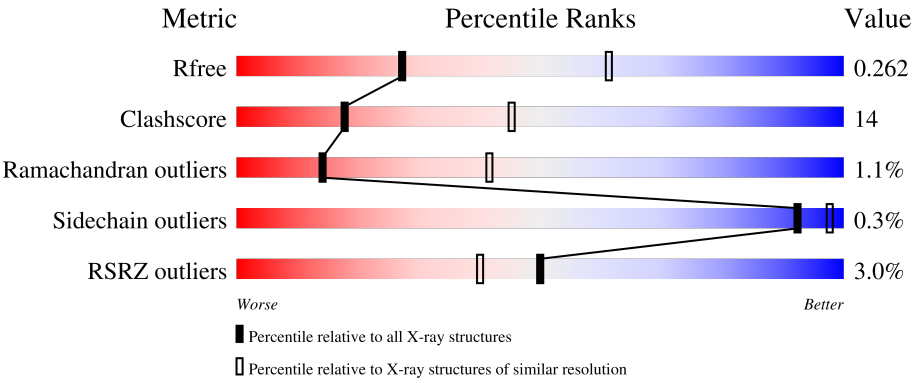
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	83% 17%
1	C	230	% 67% 26%
2	B	321	2% 58% 35%
2	D	321	7% 67% 31%

2 Entry composition (i)

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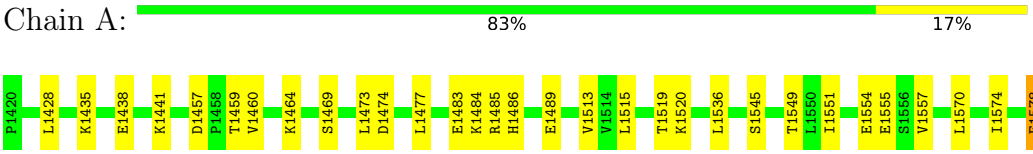
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total O 4 4	0	0
3	C	6	Total O 6 6	0	0
3	D	7	Total O 7 7	0	0

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.

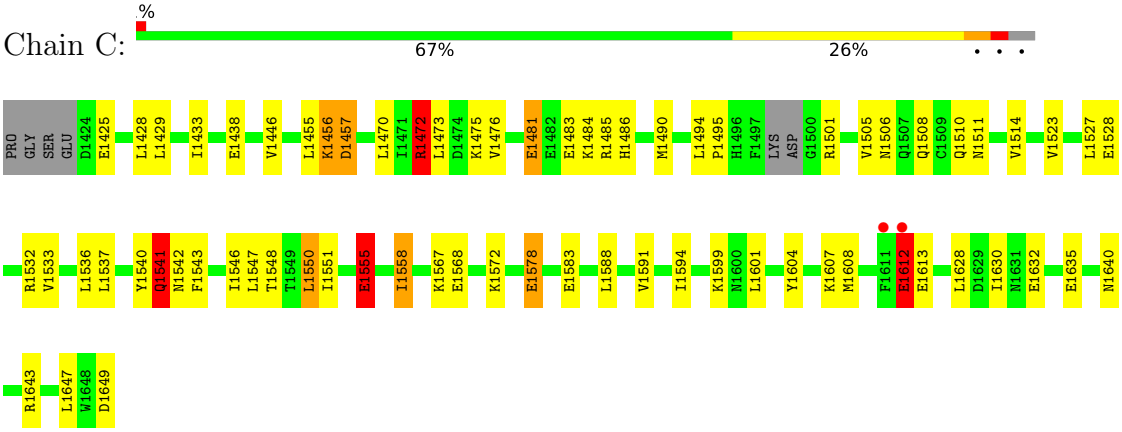
• Molecule 1: Nesprin-2

Chain A:



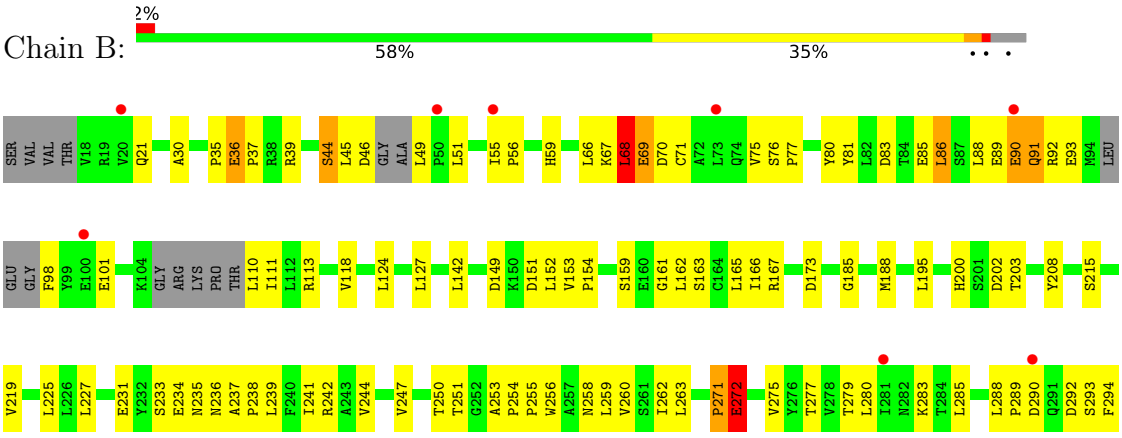
• Molecule 1: Nesprin-2

Chain C:

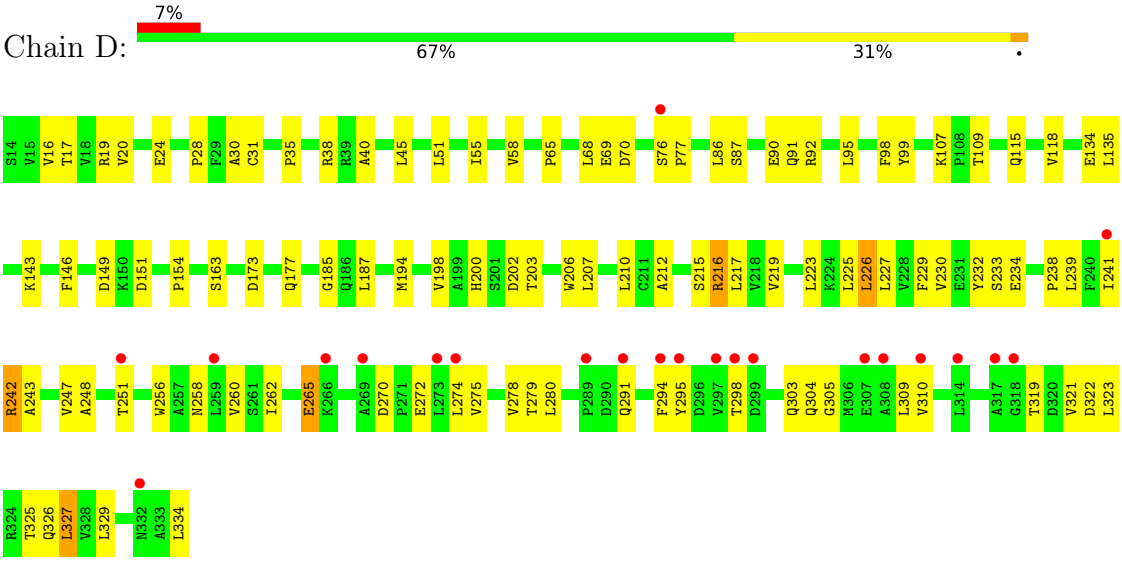


• Molecule 2: FH1/FH2 domain-containing protein 1

Chain B:



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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.08 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.262 0.218 , 0.262	Depositor DCC
R_{free} test set	1774 reflections (3.92%)	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 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	1/1920 (0.1%)	0.90	4/2584 (0.2%)
1	C	0.76	4/1865 (0.2%)	1.49	23/2514 (0.9%)
2	B	0.58	1/2404 (0.0%)	0.97	10/3276 (0.3%)
2	D	0.54	1/2510 (0.0%)	0.86	9/3424 (0.3%)
All	All	0.64	7/8699 (0.1%)	1.06	46/11798 (0.4%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1485	ARG	CB-CG	-6.99	1.33	1.52
1	C	1438	GLU	CD-OE2	6.70	1.33	1.25
2	D	35	PRO	C-N	6.63	1.49	1.34
1	C	1612	GLU	CB-CG	6.00	1.63	1.52
2	B	272	GLU	CG-CD	-5.62	1.43	1.51
1	C	1483	GLU	CD-OE2	5.53	1.31	1.25
1	C	1612	GLU	CG-CD	5.03	1.59	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1578	GLU	OE1-CD-OE2	-26.49	91.51	123.30
1	C	1555	GLU	OE1-CD-OE2	-24.94	93.38	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1472	ARG	NE-CZ-NH1	-16.57	112.02	120.30
1	C	1555	GLU	CG-CD-OE1	15.93	150.15	118.30
1	C	1578	GLU	CG-CD-OE1	15.53	149.36	118.30
1	C	1612	GLU	CA-CB-CG	14.24	144.74	113.40
2	B	86	LEU	CA-CB-CG	14.21	147.98	115.30
1	A	1485	ARG	CG-CD-NE	-13.16	84.16	111.80
1	C	1555	GLU	CG-CD-OE2	-11.60	95.10	118.30
1	C	1612	GLU	CB-CA-C	11.54	133.49	110.40
1	C	1578	GLU	CG-CD-OE2	-11.20	95.91	118.30
1	C	1472	ARG	CG-CD-NE	-11.19	88.30	111.80
1	C	1472	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	1428	LEU	CA-CB-CG	9.31	136.72	115.30
1	C	1481	GLU	CB-CA-C	-9.28	91.84	110.40
1	C	1472	ARG	CD-NE-CZ	9.06	136.28	123.60
1	C	1550	LEU	CB-CG-CD2	8.25	125.03	111.00
2	B	301	LEU	CA-CB-CG	7.97	133.63	115.30
2	D	134	GLU	CA-CB-CG	7.93	130.85	113.40
2	B	272	GLU	CA-CB-CG	7.04	128.90	113.40
1	C	1541	GLN	CA-CB-CG	7.04	128.90	113.40
1	C	1647	LEU	CA-CB-CG	6.89	131.14	115.30
2	B	283	LYS	CD-CE-NZ	-6.75	96.17	111.70
2	D	68	LEU	CB-CG-CD2	-6.64	99.72	111.00
1	C	1475	LYS	CA-CB-CG	6.46	127.61	113.40
2	D	216	ARG	CB-CA-C	6.41	123.21	110.40
1	C	1425	GLU	CA-CB-CG	6.33	127.32	113.40
1	C	1612	GLU	C-N-CA	6.32	137.50	121.70
2	B	327	LEU	CB-CG-CD1	-6.20	100.45	111.00
2	D	327	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	C	1455	LEU	C-N-CA	6.08	136.90	121.70
2	B	36	GLU	CA-CB-CG	-6.08	100.04	113.40
1	A	1485	ARG	CB-CG-CD	6.01	127.23	111.60
2	B	68	LEU	CA-CB-CG	-5.95	101.61	115.30
1	C	1541	GLN	CB-CA-C	-5.83	98.74	110.40
2	B	173	ASP	CB-CG-OD2	5.80	123.52	118.30
2	D	242	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	D	329	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	C	1612	GLU	CG-CD-OE2	5.55	129.40	118.30
2	D	242	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	D	226	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	C	1475	LYS	CG-CD-CE	5.46	128.29	111.90
2	B	272	GLU	N-CA-CB	-5.21	101.22	110.60
1	A	1578	GLU	CA-CB-CG	5.21	124.85	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	SER	C-N-CA	-5.21	108.69	121.70
2	D	143	LYS	CD-CE-NZ	-5.01	100.17	111.70

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 (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	1892	0	1906	23	0
1	C	1836	0	1834	43	0
2	B	2363	0	2347	94	0
2	D	2465	0	2469	76	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	232	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 (232) 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
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
2:B:275:VAL:O	2:B:279:THR:HG23	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:1540:TYR:O	1:C:1541:GLN:C	2.40	0.60
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:270:ASP:C	2:D:274:LEU:HD22	2.22	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:265:GLU:O	2:D:265:GLU:HG2	2.04	0.58
2:D:16:VAL:HG23	2:D:45:LEU:HB2	1.85	0.58
2:B:188:MET:HE1	2:B:225:LEU:HD22	1.86	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: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
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:279:THR:HG22	2:B:326:GLN:CD	2.24	0.56
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: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:D:272:GLU:H	2:D:272:GLU:CD	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:ARG:HH21	2:D:270:ASP:CG	2.12	0.45
2:D:226:LEU:HD23	2:D:226:LEU:HA	1.72	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: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: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:D:194:MET:HE3	2:D:229:PHE:HD1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:185:GLY:HA2	2:B:188:MET:HE2	2.03	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
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:35:PRO:C	2:B:36:GLU:HG2	2.40	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%)	5	17
2	B	299/321 (93%)	281 (94%)	13 (4%)	5 (2%)	9	29
2	D	319/321 (99%)	309 (97%)	9 (3%)	1 (0%)	41	72
All	All	1067/1102 (97%)	1030 (96%)	25 (2%)	12 (1%)	14	41

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
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%)	204 (99%)	2 (1%)	76	93
2	B	258/276 (94%)	257 (100%)	1 (0%)	91	97
2	D	269/276 (98%)	269 (100%)	0	100	100
All	All	947/982 (96%)	944 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	39	ARG
1	C	1484	LYS
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	1496	HIS
2	B	158	HIS
2	B	245	ASN
2	D	200	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/230 (100%)	0.06	0 100 100	48, 66, 109, 147	0
1	C	224/230 (97%)	0.08	2 (0%) 84 80	70, 92, 146, 177	0
2	B	307/321 (95%)	0.17	8 (2%) 56 46	54, 103, 171, 205	0
2	D	321/321 (100%)	0.31	22 (6%) 16 10	54, 98, 183, 232	0
All	All	1082/1102 (98%)	0.17	32 (2%) 50 40	48, 91, 170, 232	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	314	LEU	5.4
2	D	297	VAL	4.7
2	D	295	TYR	4.2
1	C	1612	GLU	3.8
2	D	317	ALA	3.4
2	D	318	GLY	3.3
2	B	90	GLU	3.1
2	D	299	ASP	3.0
2	B	281	ILE	3.0
2	B	290	ASP	3.0
2	D	259	LEU	3.0
2	B	20	VAL	2.8
2	D	308	ALA	2.7
2	D	310	VAL	2.6
2	D	298	THR	2.5
2	D	289	PRO	2.5
2	B	50	PRO	2.5
2	D	273	LEU	2.5
2	D	266	LYS	2.4
2	D	291	GLN	2.4
1	C	1611	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	251	THR	2.3
2	D	274	LEU	2.3
2	B	100	GLU	2.2
2	D	294	PHE	2.2
2	D	76	SER	2.1
2	D	241	ILE	2.1
2	D	332	ASN	2.1
2	B	55	ILE	2.1
2	D	307	GLU	2.1
2	B	73	LEU	2.0
2	D	269	ALA	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 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.