



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:17 PM EDT

PDB ID : 4FHM / pdb_00004fhm
Title : Nup37-Nup120(aa1-961) complex from Schizosaccharomyces pombe
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-06-06
Resolution : 4.34 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

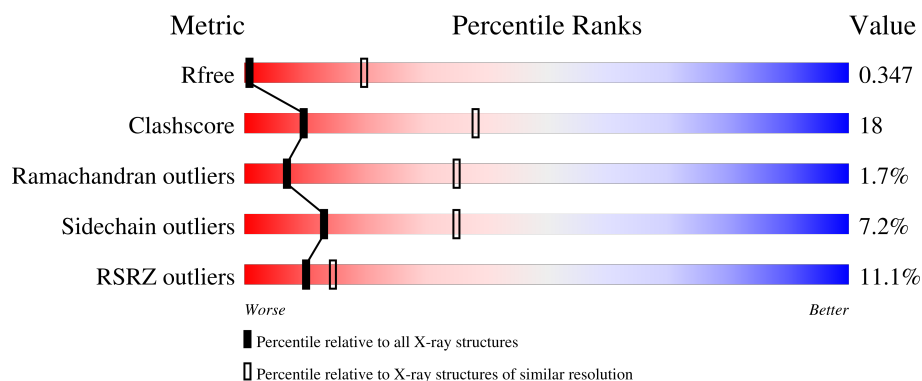
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.34 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	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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	394	9% 62% 27% 10%
2	B	964	11% 53% 37% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10113 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 NUCLEOPORIN NUP37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2718	1724	462	517	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP O36030
A	-1	GLY	-	expression tag	UNP O36030
A	0	SER	-	expression tag	UNP O36030

- Molecule 2 is a protein called Nucleoporin nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	920	Total	C	N	O	S	0	0	0
			7395	4779	1171	1418	27			

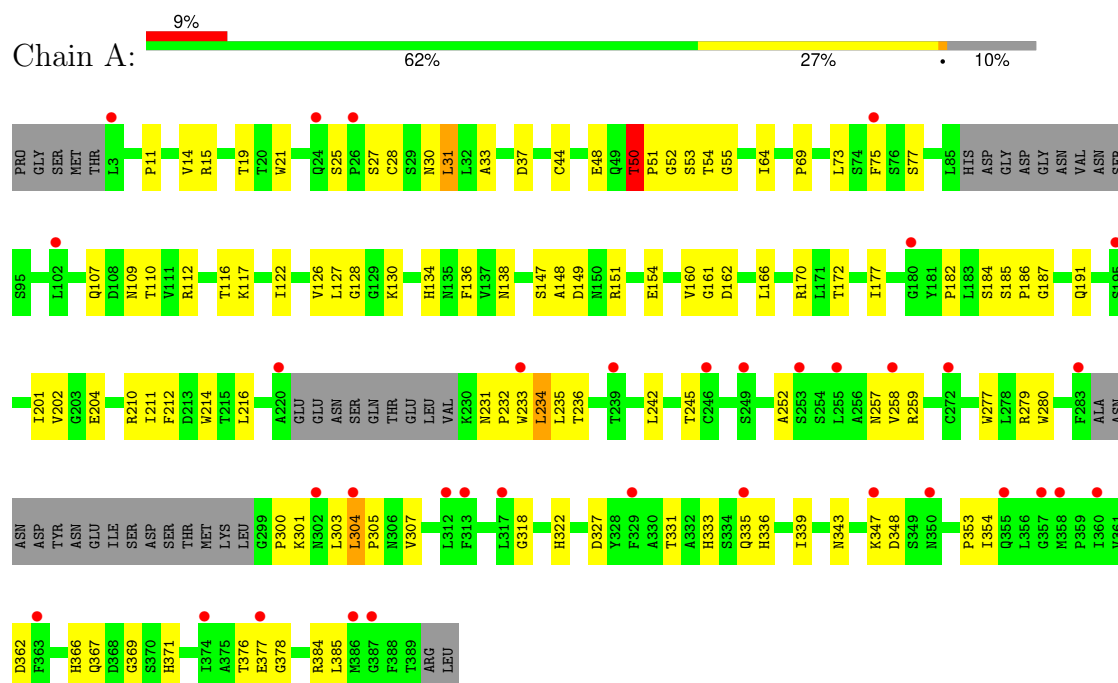
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	expression tag	UNP O43044
B	-1	GLY	-	expression tag	UNP O43044
B	0	SER	-	expression tag	UNP O43044

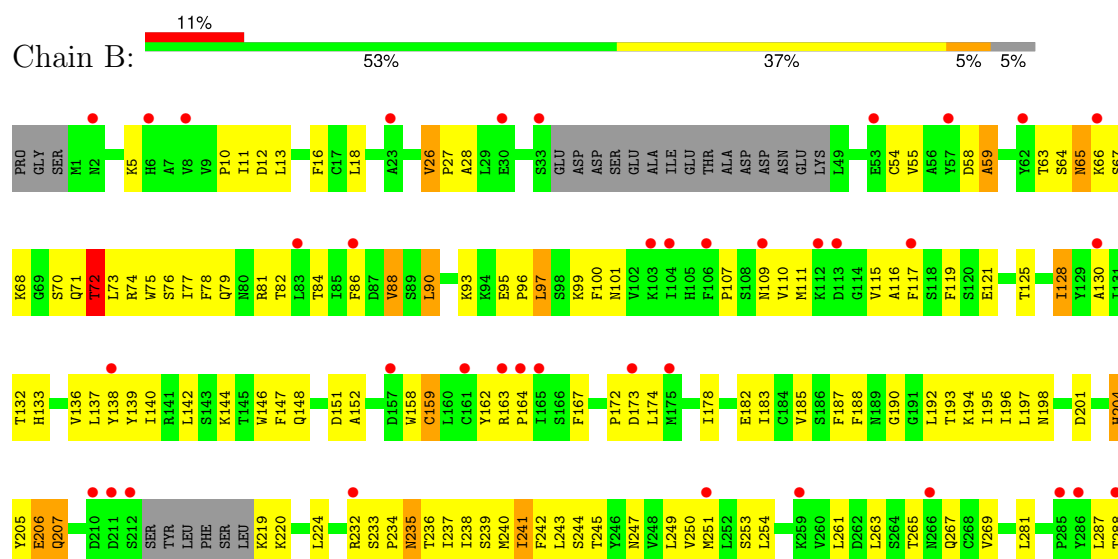
3 Residue-property plots

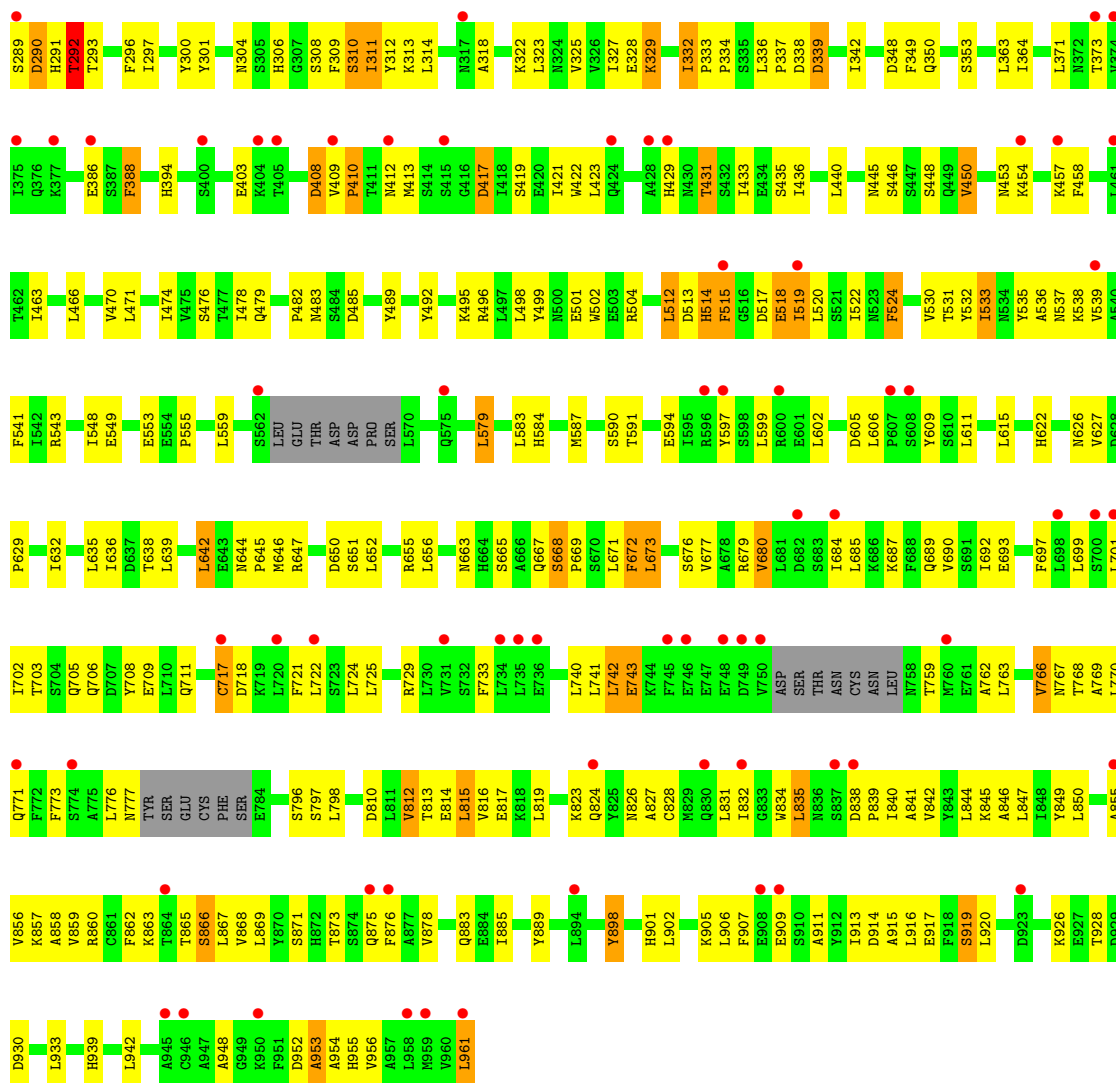
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NUCLEOPORIN NUP37



• Molecule 2: Nucleoporin nup120





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.05Å 164.05Å 310.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.50 – 4.34 64.50 – 4.34	Depositor EDS
% Data completeness (in resolution range)	99.0 (64.50-4.34) 99.0 (64.50-4.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.8_1063	Depositor
R, R_{free}	0.301 , 0.348 0.305 , 0.347	Depositor DCC
R_{free} test set	1456 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	202.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 403.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10113	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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	0.35	0/2782	0.86	3/3799 (0.1%)
2	B	0.38	0/7560	0.88	22/10259 (0.2%)
All	All	0.37	0/10342	0.88	25/14058 (0.2%)

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
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	868	VAL	N-CA-C	-11.30	102.14	113.10
1	A	50	THR	CA-C-N	-8.14	110.26	120.51
1	A	50	THR	C-N-CA	-8.14	110.26	120.51
2	B	766	VAL	N-CA-C	7.94	118.52	110.82
2	B	245	THR	N-CA-C	-6.75	103.17	111.40
2	B	409	VAL	N-CA-C	6.66	114.73	107.60
1	A	161	GLY	N-CA-C	6.37	120.40	111.10
2	B	515	PHE	N-CA-C	-6.36	106.49	114.56
2	B	514	HIS	N-CA-C	-6.14	104.96	112.88
2	B	72	THR	N-CA-C	5.80	118.30	109.95
2	B	292	THR	N-CA-C	5.78	117.89	108.76
2	B	611	LEU	N-CA-C	5.73	117.52	111.28
2	B	408	ASP	N-CA-C	5.65	117.24	111.14
2	B	668	SER	CA-C-N	5.65	126.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	668	SER	C-N-CA	5.65	126.90	119.84
2	B	204	HIS	N-CA-C	5.46	117.99	109.52
2	B	742	LEU	N-CA-C	5.33	117.91	109.96
2	B	304	ASN	N-CA-C	5.33	115.89	108.00
2	B	163	ARG	CA-C-N	5.30	126.46	119.84
2	B	163	ARG	C-N-CA	5.30	126.46	119.84
2	B	65	ASN	N-CA-C	5.28	117.00	108.34
2	B	26	VAL	CA-C-N	5.22	126.36	119.84
2	B	26	VAL	C-N-CA	5.22	126.36	119.84
2	B	386	GLU	N-CA-C	-5.18	106.91	113.18
2	B	310	SER	N-CA-C	5.08	114.54	107.73

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	THR	Peptide
2	B	206	GLU	Peptide
2	B	244	SER	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	2718	0	2670	77	0
2	B	7395	0	7319	292	0
All	All	10113	0	9989	353	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 18.

All (353) 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:64:SER:HG	2:B:76:SER:HG	1.11	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:LYS:H	2:B:96:PRO:HG3	1.43	0.84
2:B:86:PHE:HB3	2:B:101:ASN:HD22	1.45	0.82
2:B:673:LEU:HB2	2:B:770:LEU:HD22	1.62	0.82
1:A:112:ARG:HG2	1:A:126:VAL:HG13	1.64	0.79
2:B:249:LEU:HB2	2:B:261:LEU:HB3	1.64	0.79
2:B:828:CYS:HA	2:B:831:LEU:HB2	1.65	0.77
2:B:219:LYS:HD3	2:B:220:LYS:HG3	1.68	0.76
2:B:866:SER:OG	2:B:867:LEU:N	2.17	0.76
1:A:371:HIS:NE2	1:A:384:ARG:HD2	2.01	0.76
2:B:10:PRO:HB3	2:B:433:ILE:HD11	1.67	0.75
2:B:916:LEU:HD11	2:B:948:ALA:HB3	1.67	0.74
2:B:164:PRO:HG2	2:B:195:ILE:HD13	1.70	0.74
2:B:673:LEU:HD13	2:B:770:LEU:HD13	1.69	0.73
1:A:279:ARG:HB3	1:A:307:VAL:HG12	1.70	0.73
2:B:65:ASN:HB2	2:B:75:TRP:CD1	2.23	0.73
2:B:194:LYS:HB3	2:B:205:TYR:HB2	1.69	0.73
2:B:192:LEU:HD11	2:B:251:MET:SD	2.29	0.72
1:A:117:LYS:HG2	1:A:122:ILE:HD13	1.73	0.71
1:A:371:HIS:CE1	1:A:384:ARG:HD2	2.26	0.70
2:B:743:GLU:OE2	2:B:823:LYS:NZ	2.22	0.70
2:B:337:PRO:HG3	2:B:394:HIS:HE1	1.55	0.70
2:B:310:SER:OG	2:B:311:ILE:N	2.24	0.70
2:B:81:ARG:H	2:B:109:ASN:HB3	1.58	0.69
2:B:66:LYS:HG3	2:B:119:PHE:HB2	1.73	0.69
1:A:343:ASN:H	1:A:348:ASP:HB2	1.59	0.68
2:B:90:LEU:HA	2:B:669:PRO:HG3	1.75	0.68
1:A:55:GLY:H	1:A:384:ARG:HH11	1.42	0.67
2:B:313:LYS:HB3	2:B:329:LYS:HD3	1.74	0.67
2:B:555:PRO:O	2:B:559:LEU:N	2.23	0.67
2:B:79:GLN:HB3	2:B:82:THR:HB	1.74	0.67
2:B:190:GLY:HA2	2:B:236:THR:HA	1.77	0.67
1:A:252:ALA:HB2	2:B:826:ASN:HD22	1.59	0.67
2:B:729:ARG:HH12	2:B:812:VAL:HG11	1.60	0.66
2:B:871:SER:H	2:B:883:GLN:HG2	1.60	0.66
2:B:412:ASN:ND2	2:B:594:GLU:OE2	2.29	0.66
2:B:763:LEU:HD22	2:B:771:GLN:HG2	1.76	0.66
1:A:170:ARG:HD3	1:A:214:TRP:HZ3	1.60	0.66
1:A:304:LEU:HD22	1:A:305:PRO:HD2	1.77	0.65
2:B:164:PRO:HB3	2:B:204:HIS:CD2	2.32	0.65
2:B:817:GLU:HA	2:B:844:LEU:HD11	1.79	0.65
2:B:913:ILE:HA	2:B:916:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:SER:HA	2:B:332:ILE:H	1.62	0.64
2:B:533:ILE:HD12	2:B:535:TYR:HE1	1.63	0.64
2:B:28:ALA:HB1	2:B:107:PRO:HB3	1.79	0.64
2:B:839:PRO:HB2	2:B:869:LEU:HD11	1.80	0.64
2:B:78:PHE:HZ	2:B:117:PHE:HB3	1.63	0.64
1:A:202:VAL:HB	1:A:210:ARG:HB2	1.79	0.64
2:B:247:ASN:HB3	2:B:263:LEU:HD12	1.80	0.64
2:B:130:ALA:HB3	2:B:138:TYR:HB2	1.80	0.63
2:B:349:PHE:HA	2:B:522:ILE:HD11	1.80	0.63
1:A:28:CYS:HB3	1:A:31:LEU:HD22	1.79	0.63
2:B:776:LEU:HD13	2:B:797:SER:HA	1.81	0.63
2:B:435:SER:HB2	2:B:512:LEU:HB3	1.81	0.63
1:A:149:ASP:O	1:A:151:ARG:NH1	2.32	0.62
1:A:301:LYS:HD3	2:B:479:GLN:HB3	1.81	0.62
1:A:233:TRP:HD1	2:B:413:MET:SD	2.23	0.62
2:B:535:TYR:HB2	2:B:538:LYS:O	2.00	0.62
1:A:154:GLU:HG2	1:A:172:THR:HG22	1.82	0.61
2:B:815:LEU:HD22	2:B:819:LEU:HD11	1.82	0.61
2:B:646:MET:HE2	2:B:717:CYS:HB3	1.81	0.61
1:A:19:THR:HG22	1:A:362:ASP:HB3	1.81	0.60
2:B:67:SER:HB2	2:B:73:LEU:HG	1.82	0.60
2:B:240:MET:HG3	2:B:251:MET:HG2	1.82	0.60
2:B:817:GLU:OE2	2:B:876:PHE:N	2.24	0.60
1:A:170:ARG:HB2	1:A:177:ILE:HB	1.84	0.60
2:B:10:PRO:HG3	2:B:431:THR:HA	1.84	0.60
2:B:680:VAL:HG22	2:B:684:ILE:HD13	1.82	0.60
2:B:824:GLN:HG2	2:B:827:ALA:HB3	1.83	0.59
2:B:729:ARG:HH22	2:B:810:ASP:HB3	1.68	0.59
2:B:733:PHE:HA	2:B:834:TRP:CZ3	2.37	0.59
1:A:37:ASP:HA	1:A:69:PRO:HA	1.85	0.59
1:A:51:PRO:C	1:A:53:SER:H	2.10	0.59
2:B:770:LEU:O	2:B:773:PHE:N	2.35	0.59
2:B:952:ASP:HB3	2:B:955:HIS:HD2	1.68	0.58
2:B:78:PHE:HD2	2:B:110:VAL:HG21	1.69	0.58
2:B:520:LEU:HD11	2:B:536:ALA:HB2	1.85	0.58
2:B:445:ASN:HB2	2:B:448:SER:HB2	1.85	0.58
2:B:65:ASN:HB2	2:B:75:TRP:HD1	1.65	0.57
2:B:690:VAL:O	2:B:693:GLU:HB2	2.05	0.57
2:B:12:ASP:HB2	2:B:433:ILE:HG23	1.87	0.57
2:B:182:GLU:HG2	2:B:196:ILE:HG13	1.86	0.57
2:B:192:LEU:O	2:B:207:GLN:N	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:HD11	2:B:292:THR:HG22	1.86	0.57
2:B:164:PRO:HD2	2:B:167:PHE:HE1	1.70	0.57
1:A:109:ASN:OD1	1:A:136:PHE:HA	2.04	0.57
2:B:293:THR:HG23	2:B:353:SER:H	1.68	0.57
2:B:835:LEU:HD21	2:B:841:ALA:HB1	1.86	0.56
1:A:136:PHE:CG	2:B:857:LYS:HG2	2.41	0.56
2:B:100:PHE:HE1	2:B:147:PHE:HA	1.69	0.56
2:B:708:TYR:HA	2:B:711:GLN:HG3	1.88	0.56
1:A:110:THR:HG22	1:A:128:GLY:HA3	1.86	0.56
1:A:170:ARG:HD3	1:A:214:TRP:CZ3	2.41	0.56
1:A:231:ASN:HD22	1:A:232:PRO:HD2	1.69	0.56
1:A:166:LEU:HD22	1:A:202:VAL:HG21	1.86	0.55
2:B:13:LEU:HA	2:B:16:PHE:HD2	1.71	0.55
1:A:25:SER:HB2	1:A:77:SER:HA	1.88	0.55
2:B:615:LEU:O	2:B:699:LEU:HD13	2.07	0.55
1:A:212:PHE:HD1	1:A:233:TRP:HB3	1.71	0.54
2:B:74:ARG:HH22	2:B:144:LYS:HG2	1.72	0.54
2:B:72:THR:HG21	2:B:144:LYS:HE3	1.90	0.54
2:B:668:SER:HB2	2:B:672:PHE:HD2	1.72	0.54
2:B:288:THR:OG1	2:B:348:ASP:OD1	2.18	0.54
2:B:269:VAL:HG23	2:B:322:LYS:HE2	1.90	0.54
2:B:729:ARG:NH1	2:B:812:VAL:HG11	2.23	0.53
2:B:501:GLU:OE1	2:B:504:ARG:NH2	2.41	0.53
2:B:873:THR:HG22	2:B:883:GLN:HE22	1.73	0.53
2:B:915:ALA:O	2:B:919:SER:OG	2.24	0.53
2:B:768:THR:C	2:B:770:LEU:H	2.15	0.53
2:B:373:THR:HG21	2:B:519:ILE:HG21	1.90	0.53
2:B:693:GLU:HB3	2:B:697:PHE:CZ	2.44	0.53
2:B:311:ILE:HB	2:B:332:ILE:HG13	1.89	0.53
2:B:77:ILE:O	2:B:84:THR:OG1	2.22	0.52
2:B:86:PHE:HB3	2:B:101:ASN:ND2	2.19	0.52
2:B:463:ILE:HA	2:B:466:LEU:HG	1.90	0.52
2:B:665:SER:HB3	2:B:777:ASN:HB3	1.91	0.52
2:B:422:TRP:CZ2	2:B:499:TYR:HA	2.44	0.52
2:B:646:MET:SD	2:B:646:MET:N	2.82	0.52
2:B:18:LEU:HD13	2:B:101:ASN:HB2	1.91	0.52
2:B:629:PRO:HA	2:B:632:ILE:HD12	1.90	0.52
2:B:635:LEU:O	2:B:639:LEU:HG	2.10	0.52
2:B:173:ASP:HB2	2:B:188:PHE:CE1	2.45	0.52
2:B:913:ILE:O	2:B:916:LEU:HB2	2.10	0.52
2:B:454:LYS:HD2	2:B:457:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:930:ASP:HB2	2:B:933:LEU:HB3	1.91	0.52
2:B:584:HIS:HB2	2:B:693:GLU:HG2	1.92	0.52
2:B:314:LEU:HD21	2:B:325:VAL:HG13	1.92	0.51
2:B:482:PRO:HA	2:B:489:TYR:HA	1.92	0.51
2:B:816:VAL:HG12	2:B:844:LEU:HD13	1.91	0.51
2:B:741:LEU:HD23	2:B:768:THR:HG22	1.92	0.51
2:B:906:LEU:HD22	2:B:914:ASP:HB2	1.93	0.51
1:A:333:HIS:HD2	1:A:336:HIS:H	1.58	0.51
2:B:265:THR:HG22	2:B:267:GLN:HB3	1.92	0.51
2:B:518:GLU:O	2:B:536:ALA:N	2.30	0.51
2:B:838:ASP:H	2:B:841:ALA:HB3	1.75	0.51
2:B:132:THR:OG1	2:B:136:VAL:HG22	2.11	0.51
2:B:97:LEU:O	2:B:99:LYS:HG2	2.11	0.51
2:B:689:GLN:O	2:B:693:GLU:HG3	2.12	0.50
2:B:178:ILE:HD11	2:B:182:GLU:HB2	1.93	0.50
2:B:314:LEU:HD11	2:B:325:VAL:HG13	1.93	0.50
2:B:832:ILE:HG13	2:B:835:LEU:HD22	1.91	0.50
2:B:68:LYS:HG3	2:B:121:GLU:HG2	1.93	0.50
2:B:116:ALA:O	2:B:130:ALA:HA	2.11	0.50
2:B:419:SER:HB2	2:B:471:LEU:HD21	1.92	0.50
2:B:812:VAL:HG21	2:B:835:LEU:HB2	1.93	0.50
1:A:257:ASN:HB2	1:A:318:GLY:HA3	1.93	0.50
2:B:78:PHE:CZ	2:B:117:PHE:HB3	2.45	0.50
1:A:242:LEU:HD13	1:A:305:PRO:HG3	1.93	0.50
2:B:364:ILE:HG23	2:B:522:ILE:HD12	1.94	0.50
2:B:237:ILE:HA	2:B:253:SER:HA	1.94	0.49
2:B:247:ASN:HB3	2:B:263:LEU:HB2	1.95	0.49
2:B:642:LEU:HD23	2:B:645:PRO:HB3	1.94	0.49
2:B:639:LEU:HD13	2:B:701:LEU:HB3	1.93	0.49
1:A:130:LYS:O	1:A:134:HIS:NE2	2.37	0.49
1:A:160:VAL:HB	1:A:187:GLY:HA3	1.92	0.49
2:B:332:ILE:HG12	2:B:388:PHE:HE2	1.77	0.49
2:B:63:THR:HB	2:B:75:TRP:HZ2	1.77	0.49
2:B:12:ASP:HB2	2:B:433:ILE:CG2	2.42	0.49
1:A:339:ILE:HB	1:A:354:ILE:HB	1.95	0.49
2:B:233:SER:O	2:B:235:ASN:N	2.43	0.49
2:B:587:MET:HG2	2:B:591:THR:HG21	1.94	0.49
2:B:926:LYS:NZ	2:B:930:ASP:H	2.10	0.49
2:B:650:ASP:OD1	2:B:651:SER:N	2.45	0.49
2:B:952:ASP:HB3	2:B:955:HIS:CD2	2.46	0.49
1:A:107:GLN:HA	2:B:860:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HB2	2:B:669:PRO:HA	1.95	0.48
2:B:478:ILE:HD11	2:B:501:GLU:HG2	1.94	0.48
2:B:768:THR:OG1	2:B:769:ALA:N	2.46	0.48
2:B:193:THR:HA	2:B:206:GLU:HA	1.95	0.48
1:A:191:GLN:OE1	1:A:259:ARG:HD2	2.13	0.48
2:B:842:VAL:HG11	2:B:865:THR:HG21	1.94	0.48
2:B:863:LYS:HZ3	2:B:961:LEU:HA	1.79	0.48
2:B:59:ALA:O	2:B:536:ALA:HB1	2.13	0.48
2:B:137:LEU:HB2	2:B:162:TYR:O	2.12	0.48
2:B:767:ASN:HB3	2:B:770:LEU:HD21	1.96	0.48
2:B:953:ALA:C	2:B:955:HIS:H	2.22	0.48
1:A:107:GLN:HE22	2:B:860:ARG:HG2	1.78	0.48
2:B:767:ASN:HB3	2:B:770:LEU:HD11	1.94	0.48
1:A:210:ARG:HH12	2:B:417:ASP:H	1.61	0.48
2:B:12:ASP:H	2:B:433:ILE:HG13	1.79	0.48
2:B:840:ILE:HG12	2:B:875:GLN:HE21	1.79	0.48
2:B:88:VAL:HB	2:B:671:LEU:HD22	1.95	0.47
2:B:128:ILE:CG2	2:B:140:ILE:HB	2.43	0.47
2:B:632:ILE:O	2:B:636:ILE:HG12	2.14	0.47
2:B:536:ALA:O	2:B:538:LYS:HD2	2.14	0.47
2:B:72:THR:OG1	2:B:73:LEU:N	2.45	0.47
2:B:590:SER:O	2:B:594:GLU:HG2	2.15	0.47
2:B:639:LEU:HD22	2:B:701:LEU:HD13	1.96	0.47
2:B:332:ILE:HG12	2:B:388:PHE:CE2	2.49	0.47
2:B:192:LEU:HB2	2:B:207:GLN:CG	2.45	0.47
2:B:235:ASN:O	2:B:235:ASN:ND2	2.45	0.47
1:A:130:LYS:HD3	2:B:609:TYR:HE1	1.80	0.47
2:B:519:ILE:HA	2:B:535:TYR:HA	1.96	0.47
2:B:636:ILE:HA	2:B:639:LEU:HD12	1.96	0.47
2:B:797:SER:OG	2:B:798:LEU:N	2.46	0.47
2:B:466:LEU:O	2:B:470:VAL:HG23	2.15	0.46
2:B:599:LEU:HA	2:B:602:LEU:HB2	1.97	0.46
2:B:174:LEU:HD21	2:B:240:MET:H	1.79	0.46
1:A:184:SER:OG	1:A:204:GLU:OE1	2.32	0.46
1:A:147:SER:OG	1:A:148:ALA:N	2.49	0.46
1:A:53:SER:OG	1:A:54:THR:N	2.38	0.46
1:A:211:ILE:O	1:A:234:LEU:HB2	2.15	0.46
1:A:236:THR:HB	2:B:417:ASP:HB3	1.97	0.46
1:A:51:PRO:O	1:A:53:SER:N	2.45	0.46
1:A:212:PHE:CD1	1:A:233:TRP:HB3	2.50	0.46
2:B:178:ILE:HG21	2:B:263:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:ASN:HD22	2:B:647:ARG:HB2	1.80	0.46
2:B:849:TYR:HB3	2:B:858:ALA:HB2	1.97	0.46
1:A:233:TRP:CE3	1:A:233:TRP:HA	2.51	0.46
2:B:243:LEU:HD11	2:B:292:THR:OG1	2.15	0.46
2:B:599:LEU:HD23	2:B:602:LEU:HD12	1.96	0.46
1:A:51:PRO:C	1:A:53:SER:N	2.74	0.46
2:B:111:MET:HA	2:B:133:HIS:HA	1.98	0.46
2:B:140:ILE:HG23	2:B:158:TRP:HD1	1.79	0.45
2:B:549:GLU:O	2:B:553:GLU:HG2	2.16	0.45
2:B:306:HIS:ND1	2:B:308:SER:HB3	2.31	0.45
2:B:318:ALA:HA	2:B:323:LEU:HA	1.98	0.45
2:B:815:LEU:HD23	2:B:815:LEU:HA	1.81	0.45
2:B:855:ALA:O	2:B:859:VAL:HG23	2.16	0.45
2:B:314:LEU:HG	2:B:327:ILE:HG12	1.97	0.45
2:B:579:LEU:O	2:B:583:LEU:HG	2.16	0.45
2:B:72:THR:HB	2:B:93:LYS:NZ	2.31	0.45
2:B:530:VAL:HB	2:B:541:PHE:CZ	2.51	0.45
2:B:142:LEU:HD22	2:B:146:TRP:CZ3	2.52	0.45
2:B:636:ILE:HD13	2:B:639:LEU:HD12	2.00	0.44
1:A:303:LEU:HD21	2:B:479:GLN:HA	2.00	0.44
2:B:71:GLN:HB3	2:B:93:LYS:HE2	1.98	0.44
2:B:172:PRO:HA	2:B:187:PHE:HD1	1.82	0.44
2:B:241:ILE:HG22	2:B:250:VAL:HB	1.98	0.44
2:B:220:LYS:O	2:B:224:LEU:HG	2.18	0.44
2:B:54:CYS:SG	2:B:55:VAL:N	2.90	0.44
2:B:453:ASN:O	2:B:457:LYS:HG3	2.17	0.44
2:B:846:ALA:HB1	2:B:862:PHE:CZ	2.52	0.44
2:B:192:LEU:HB2	2:B:207:GLN:HG3	2.00	0.44
1:A:280:TRP:CD1	1:A:305:PRO:HA	2.52	0.44
2:B:312:TYR:HD2	2:B:327:ILE:HG21	1.83	0.44
2:B:533:ILE:HD12	2:B:535:TYR:CE1	2.48	0.44
2:B:121:GLU:HB2	2:B:125:THR:O	2.18	0.44
2:B:198:ASN:HB3	2:B:201:ASP:HB2	2.00	0.44
2:B:242:PHE:HD1	2:B:249:LEU:HD13	1.81	0.44
2:B:718:ASP:O	2:B:722:LEU:HG	2.18	0.44
1:A:162:ASP:OD1	1:A:186:PRO:HB3	2.18	0.44
2:B:311:ILE:HD11	2:B:363:LEU:HD22	2.00	0.44
2:B:498:LEU:O	2:B:502:TRP:HD1	2.00	0.44
2:B:665:SER:CB	2:B:777:ASN:HB3	2.48	0.44
2:B:697:PHE:O	2:B:701:LEU:HG	2.18	0.44
2:B:905:LYS:O	2:B:909:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:ALA:O	2:B:955:HIS:N	2.50	0.43
1:A:21:TRP:CH2	1:A:366:HIS:HD2	2.36	0.43
2:B:602:LEU:HD22	2:B:606:LEU:HB2	1.99	0.43
2:B:676:SER:O	2:B:680:VAL:HB	2.17	0.43
2:B:436:ILE:O	2:B:440:LEU:HG	2.18	0.43
2:B:706:GLN:HA	2:B:709:GLU:CD	2.43	0.43
1:A:30:ASN:O	1:A:44:CYS:HA	2.19	0.43
2:B:939:HIS:O	2:B:942:LEU:HB2	2.18	0.43
2:B:885:ILE:HD12	2:B:901:HIS:ND1	2.33	0.43
1:A:64:ILE:HD13	1:A:116:THR:HG21	2.01	0.43
1:A:322:HIS:NE2	1:A:369:GLY:O	2.36	0.43
2:B:651:SER:O	2:B:655:ARG:HG3	2.19	0.43
2:B:898:TYR:CD1	2:B:898:TYR:C	2.96	0.43
2:B:151:ASP:OD1	2:B:152:ALA:N	2.51	0.43
2:B:241:ILE:CG2	2:B:250:VAL:HB	2.48	0.43
2:B:622:HIS:O	2:B:627:VAL:HG21	2.19	0.43
2:B:847:LEU:O	2:B:850:LEU:HB2	2.19	0.43
2:B:741:LEU:HA	2:B:768:THR:HB	2.01	0.43
2:B:859:VAL:HG12	2:B:863:LYS:HE3	1.99	0.43
1:A:335:GLN:HG3	1:A:336:HIS:CD2	2.54	0.43
2:B:652:LEU:HD23	2:B:655:ARG:NE	2.34	0.43
2:B:889:TYR:CG	2:B:933:LEU:HD13	2.53	0.43
1:A:138:ASN:HD21	1:A:162:ASP:CG	2.27	0.43
1:A:236:THR:HG21	2:B:417:ASP:OD1	2.18	0.43
2:B:136:VAL:HG23	2:B:138:TYR:HE1	1.84	0.43
2:B:417:ASP:OD1	2:B:417:ASP:N	2.52	0.43
2:B:743:GLU:HG2	2:B:766:VAL:HG23	2.01	0.43
2:B:917:GLU:O	2:B:920:LEU:HB2	2.18	0.43
1:A:277:TRP:HZ3	1:A:307:VAL:HG13	1.84	0.42
2:B:705:GLN:O	2:B:709:GLU:HG3	2.19	0.42
2:B:64:SER:OG	2:B:76:SER:OG	1.97	0.42
2:B:454:LYS:HD2	2:B:454:LYS:HA	1.86	0.42
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.60	0.42
2:B:243:LEU:HD23	2:B:243:LEU:HA	1.88	0.42
2:B:740:LEU:HD13	2:B:827:ALA:HB1	2.00	0.42
1:A:107:GLN:NE2	2:B:860:ARG:HG2	2.35	0.42
1:A:211:ILE:HD12	1:A:235:LEU:HD23	2.02	0.42
2:B:142:LEU:HD22	2:B:146:TRP:CE3	2.54	0.42
2:B:290:ASP:OD1	2:B:290:ASP:N	2.52	0.42
2:B:543:ARG:HB3	2:B:679:ARG:HH12	1.84	0.42
2:B:652:LEU:HD23	2:B:655:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:718:ASP:O	2:B:721:PHE:HB3	2.19	0.42
2:B:724:LEU:HD23	2:B:724:LEU:HA	1.93	0.42
2:B:845:LYS:O	2:B:849:TYR:HD2	2.01	0.42
1:A:11:PRO:HB2	1:A:14:VAL:HG23	2.02	0.42
1:A:212:PHE:CE2	1:A:214:TRP:HB3	2.55	0.42
2:B:663:ASN:OD1	2:B:796:SER:OG	2.35	0.42
2:B:584:HIS:CB	2:B:693:GLU:HG2	2.50	0.42
2:B:840:ILE:HG23	2:B:875:GLN:HE21	1.84	0.42
1:A:201:ILE:HA	1:A:210:ARG:O	2.20	0.42
2:B:812:VAL:CG2	2:B:835:LEU:HB2	2.50	0.42
2:B:95:GLU:O	2:B:148:GLN:NE2	2.53	0.42
2:B:350:GLN:O	2:B:363:LEU:HD12	2.20	0.42
2:B:742:LEU:HD13	2:B:826:ASN:ND2	2.35	0.42
2:B:759:THR:O	2:B:762:ALA:HB3	2.19	0.42
2:B:926:LYS:HZ2	2:B:933:LEU:HD23	1.85	0.42
2:B:638:THR:O	2:B:642:LEU:HD13	2.20	0.41
1:A:182:PRO:HB3	2:B:597:TYR:CZ	2.55	0.41
2:B:71:GLN:HB3	2:B:93:LYS:HZ1	1.85	0.41
2:B:75:TRP:HE3	2:B:86:PHE:CZ	2.39	0.41
2:B:139:TYR:O	2:B:159:CYS:HA	2.19	0.41
2:B:174:LEU:HD23	2:B:237:ILE:HD11	2.01	0.41
2:B:485:ASP:OD1	2:B:485:ASP:N	2.43	0.41
2:B:828:CYS:O	2:B:832:ILE:HB	2.20	0.41
1:A:48:GLU:OE2	1:A:50:THR:HG23	2.20	0.41
1:A:327:ASP:O	1:A:343:ASN:HA	2.20	0.41
2:B:332:ILE:HA	2:B:333:PRO:HD3	1.89	0.41
1:A:55:GLY:H	1:A:384:ARG:NH1	2.12	0.41
2:B:26:VAL:HG11	2:B:138:TYR:CE2	2.55	0.41
2:B:814:GLU:O	2:B:817:GLU:HB3	2.20	0.41
2:B:889:TYR:CD1	2:B:933:LEU:HD13	2.56	0.41
2:B:238:ILE:HG23	2:B:239:SER:H	1.85	0.41
2:B:328:GLU:C	2:B:329:LYS:HZ2	2.28	0.41
1:A:28:CYS:O	1:A:31:LEU:HB2	2.20	0.41
2:B:492:TYR:OH	2:B:496:ARG:NH2	2.53	0.41
2:B:677:VAL:O	2:B:680:VAL:HG12	2.20	0.41
2:B:5:LYS:HE2	2:B:549:GLU:HG3	2.02	0.41
2:B:233:SER:C	2:B:254:LEU:HD23	2.45	0.41
2:B:371:LEU:HG	2:B:514:HIS:O	2.21	0.41
2:B:445:ASN:OD1	2:B:446:SER:N	2.53	0.41
1:A:15:ARG:NH1	2:B:914:ASP:OD1	2.50	0.41
1:A:33:ALA:HB2	1:A:75:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:ILE:H	2:B:421:ILE:HG13	1.68	0.41
2:B:300:TYR:CD2	2:B:309:PHE:HB3	2.55	0.41
2:B:329:LYS:NZ	2:B:329:LYS:HB3	2.36	0.41
2:B:450:VAL:O	2:B:454:LYS:N	2.43	0.41
2:B:454:LYS:HG3	2:B:458:PHE:CE2	2.56	0.41
2:B:524:PHE:CE1	2:B:531:THR:HA	2.56	0.41
2:B:838:ASP:O	2:B:842:VAL:N	2.53	0.41
2:B:926:LYS:HZ1	2:B:928:THR:HB	1.84	0.41
1:A:233:TRP:HA	1:A:233:TRP:HE3	1.86	0.41
1:A:343:ASN:CG	1:A:347:LYS:HB2	2.46	0.41
2:B:339:ASP:O	2:B:342:ILE:HB	2.20	0.41
2:B:408:ASP:O	2:B:410:PRO:HD3	2.21	0.41
2:B:850:LEU:HD23	2:B:850:LEU:HA	1.86	0.40
2:B:174:LEU:HD21	2:B:240:MET:HB2	2.03	0.40
2:B:840:ILE:HG12	2:B:875:GLN:NE2	2.36	0.40
2:B:909:GLU:C	2:B:911:ALA:H	2.29	0.40
2:B:445:ASN:O	2:B:448:SER:OG	2.30	0.40
2:B:548:ILE:HD13	2:B:687:LYS:HD2	2.03	0.40
2:B:768:THR:C	2:B:770:LEU:N	2.79	0.40
1:A:134:HIS:HB3	2:B:605:ASP:OD1	2.22	0.40
1:A:303:LEU:HB3	2:B:476:SER:HA	2.03	0.40
1:A:353:PRO:HB2	1:A:385:LEU:HD22	2.03	0.40
1:A:376:THR:O	1:A:378:GLY:N	2.55	0.40
2:B:185:VAL:HB	2:B:193:THR:HG22	2.03	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	346/394 (88%)	319 (92%)	22 (6%)	5 (1%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	908/964 (94%)	771 (85%)	121 (13%)	16 (2%)	6	33
All	All	1254/1358 (92%)	1090 (87%)	143 (11%)	21 (2%)	7	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
2	B	953	ALA
1	A	50	THR
2	B	59	ALA
2	B	410	PRO
2	B	815	LEU
2	B	856	VAL
2	B	954	ALA
2	B	287	LEU
2	B	403	GLU
2	B	495	LYS
2	B	517	ASP
2	B	626	ASN
1	A	377	GLU
2	B	115	VAL
2	B	234	PRO
1	A	52	GLY
2	B	70	SER
2	B	27	PRO
1	A	300	PRO
2	B	334	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	309/345 (90%)	297 (96%)	12 (4%)	28	50
2	B	845/886 (95%)	774 (92%)	71 (8%)	10	30
All	All	1154/1231 (94%)	1071 (93%)	83 (7%)	13	35

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	31	LEU
1	A	50	THR
1	A	73	LEU
1	A	127	LEU
1	A	185	SER
1	A	216	LEU
1	A	245	THR
1	A	258	VAL
1	A	304	LEU
1	A	331	THR
1	A	367	GLN
2	B	11	ILE
2	B	58	ASP
2	B	72	THR
2	B	88	VAL
2	B	90	LEU
2	B	97	LEU
2	B	128	ILE
2	B	159	CYS
2	B	183	ILE
2	B	197	LEU
2	B	207	GLN
2	B	232	ARG
2	B	235	ASN
2	B	241	ILE
2	B	281	LEU
2	B	289	SER
2	B	290	ASP
2	B	291	HIS
2	B	292	THR
2	B	296	PHE
2	B	297	ILE
2	B	301	TYR
2	B	311	ILE
2	B	329	LYS
2	B	332	ILE
2	B	336	LEU
2	B	338	ASP
2	B	339	ASP
2	B	388	PHE
2	B	417	ASP

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Mol	Chain	Res	Type
2	B	423	LEU
2	B	429	HIS
2	B	431	THR
2	B	450	VAL
2	B	474	ILE
2	B	483	ASN
2	B	512	LEU
2	B	513	ASP
2	B	515	PHE
2	B	518	GLU
2	B	519	ILE
2	B	524	PHE
2	B	532	TYR
2	B	533	ILE
2	B	537	ASN
2	B	539	VAL
2	B	579	LEU
2	B	642	LEU
2	B	656	LEU
2	B	667	GLN
2	B	672	PHE
2	B	673	LEU
2	B	680	VAL
2	B	685	LEU
2	B	692	ILE
2	B	702	ILE
2	B	703	THR
2	B	717	CYS
2	B	725	LEU
2	B	743	GLU
2	B	812	VAL
2	B	813	THR
2	B	835	LEU
2	B	866	SER
2	B	878	VAL
2	B	898	TYR
2	B	902	LEU
2	B	907	PHE
2	B	919	SER
2	B	956	VAL
2	B	961	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	257	ASN
1	A	336	HIS
2	B	71	GLN
2	B	101	ASN
2	B	198	ASN
2	B	394	HIS
2	B	479	GLN
2	B	584	HIS
2	B	604	GLN
2	B	777	ASN
2	B	955	HIS

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	354/394 (89%)	0.70	35 (9%)	13 17	177, 274, 456, 701	0
2	B	920/964 (95%)	0.80	106 (11%)	9 13	150, 305, 521, 707	0
All	All	1274/1358 (93%)	0.77	141 (11%)	10 14	150, 298, 511, 707	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	288	THR	9.6
1	A	350	ASN	6.7
2	B	117	PHE	6.0
2	B	682	ASP	6.0
1	A	249	SER	6.0
2	B	164	PRO	5.9
2	B	700	SER	5.6
2	B	428	ALA	5.1
1	A	357	GLY	5.0
1	A	312	LEU	4.9
1	A	180	GLY	4.8
2	B	600	ARG	4.7
1	A	3	LEU	4.6
2	B	837	SER	4.5
2	B	286	TYR	4.4
2	B	113	ASP	4.1
2	B	875	GLN	4.0
2	B	33	SER	4.0
2	B	864	THR	3.8
2	B	701	LEU	3.8
2	B	608	SER	3.7
2	B	745	PHE	3.7
2	B	838	ASP	3.7
1	A	253	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLN	3.6
2	B	684	ILE	3.6
2	B	57	TYR	3.6
2	B	103	LYS	3.5
2	B	946	CYS	3.5
2	B	377	LYS	3.5
2	B	23	ALA	3.4
2	B	597	TYR	3.4
2	B	950	LYS	3.4
2	B	457	LYS	3.3
1	A	317	LEU	3.3
2	B	722	LEU	3.2
1	A	374	ILE	3.2
2	B	138	TYR	3.2
2	B	746	GLU	3.2
2	B	232	ARG	3.2
2	B	698	LEU	3.2
2	B	824	GLN	3.2
1	A	363	PHE	3.2
2	B	409	VAL	3.2
2	B	909	GLU	3.2
1	A	377	GLU	3.1
1	A	304	LEU	3.1
2	B	923	ASP	3.0
2	B	771	GLN	3.0
1	A	255	LEU	3.0
2	B	112	LYS	3.0
1	A	239	THR	2.9
2	B	83	LEU	2.9
2	B	415	SER	2.9
2	B	86	PHE	2.9
2	B	596	ARG	2.8
2	B	66	LYS	2.8
2	B	429	HIS	2.8
2	B	405	THR	2.8
2	B	894	LEU	2.8
1	A	233	TRP	2.8
2	B	412	ASN	2.8
2	B	774	SER	2.8
2	B	575	GLN	2.8
2	B	106	PHE	2.7
2	B	173	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	259	LYS	2.7
2	B	830	GLN	2.7
2	B	461	LEU	2.7
2	B	515	PHE	2.6
2	B	130	ALA	2.6
2	B	109	ASN	2.6
2	B	210	ASP	2.5
2	B	161	CYS	2.5
2	B	175	MET	2.5
2	B	607	PRO	2.5
2	B	717	CYS	2.5
2	B	157	ASP	2.5
2	B	285	PRO	2.5
2	B	945	ALA	2.5
2	B	734	LEU	2.4
2	B	212	SER	2.4
2	B	424	GLN	2.4
2	B	519	ILE	2.4
2	B	760	MET	2.4
2	B	165	ILE	2.4
2	B	832	ILE	2.4
2	B	731	VAL	2.4
2	B	454	LYS	2.4
1	A	195	SER	2.4
1	A	220	ALA	2.4
1	A	329	PHE	2.4
2	B	750	VAL	2.4
1	A	386	MET	2.4
2	B	317	ASN	2.4
1	A	283	PHE	2.3
1	A	24	GLN	2.3
2	B	961	LEU	2.3
2	B	53	GLU	2.3
1	A	272	CYS	2.3
1	A	358	MET	2.3
2	B	211	ASP	2.3
2	B	958	LEU	2.3
1	A	102	LEU	2.3
2	B	374	VAL	2.3
2	B	289	SER	2.2
1	A	258	VAL	2.2
1	A	360	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	959	MET	2.2
2	B	908	GLU	2.2
2	B	855	ALA	2.2
1	A	335	GLN	2.2
2	B	2	ASN	2.2
2	B	8	VAL	2.2
2	B	735	LEU	2.1
1	A	347	LYS	2.1
2	B	404	LYS	2.1
1	A	302	ASN	2.1
2	B	30	GLU	2.1
1	A	26	PRO	2.1
1	A	313	PHE	2.1
2	B	400	SER	2.1
2	B	562	SER	2.1
2	B	386	GLU	2.1
2	B	720	LEU	2.1
2	B	539	VAL	2.1
1	A	75	PHE	2.1
2	B	375	ILE	2.1
2	B	104	ILE	2.1
2	B	163	ARG	2.1
2	B	251	MET	2.1
2	B	62	TYR	2.1
2	B	736	GLU	2.1
2	B	749	ASP	2.0
2	B	876	PHE	2.0
1	A	246	CYS	2.0
2	B	373	THR	2.0
2	B	748	GLU	2.0
2	B	6	HIS	2.0
2	B	266	ASN	2.0
1	A	387	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.