



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:22 AM EDT

PDB ID : 1XB4 / pdb_00001xb4
Title : Crystal structure of subunit VPS25 of the endosomal trafficking complex ESCRT-II
Authors : Weissenhorn, W.; Wernimont, A.K.
Deposited on : 2004-08-27
Resolution : 3.10 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

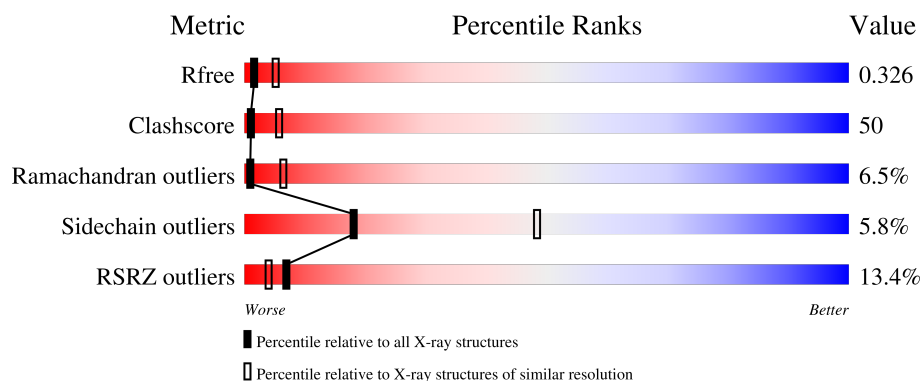
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	202	
1	B	202	
1	C	202	
1	D	202	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5773 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 Hypothetical 23.6 kDa protein in YUH1-URA8 intergenic region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1492	955	250	279	8			
1	B	179	Total	C	N	O	S	0	0	0
			1482	948	248	278	8			
1	C	180	Total	C	N	O	S	0	0	0
			1492	954	251	279	8			
1	D	154	Total	C	N	O	S	0	0	0
			1291	844	209	230	8			

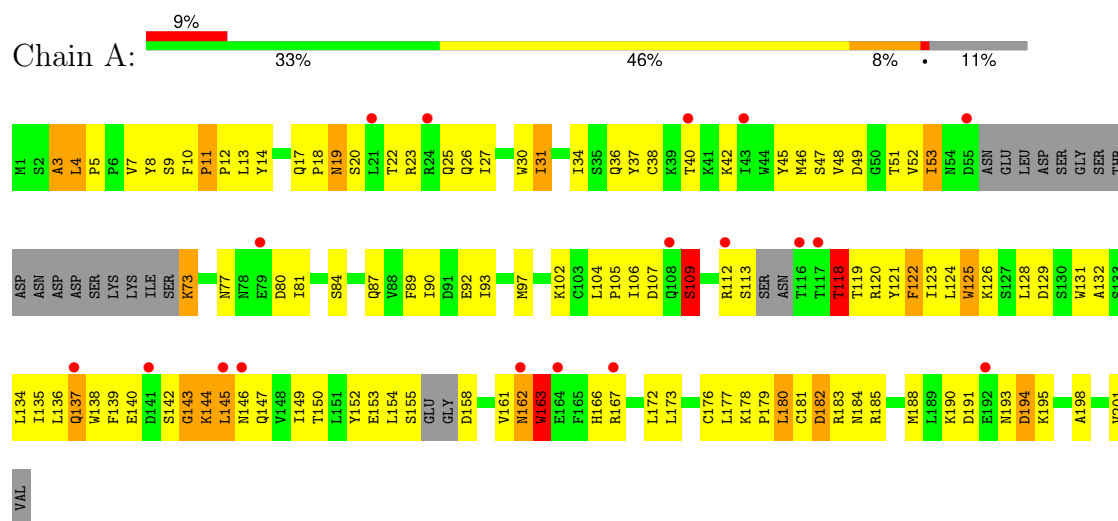
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	2	Total	O	0	0
			2	2		
2	C	7	Total	O	0	0
			7	7		
2	D	2	Total	O	0	0
			2	2		

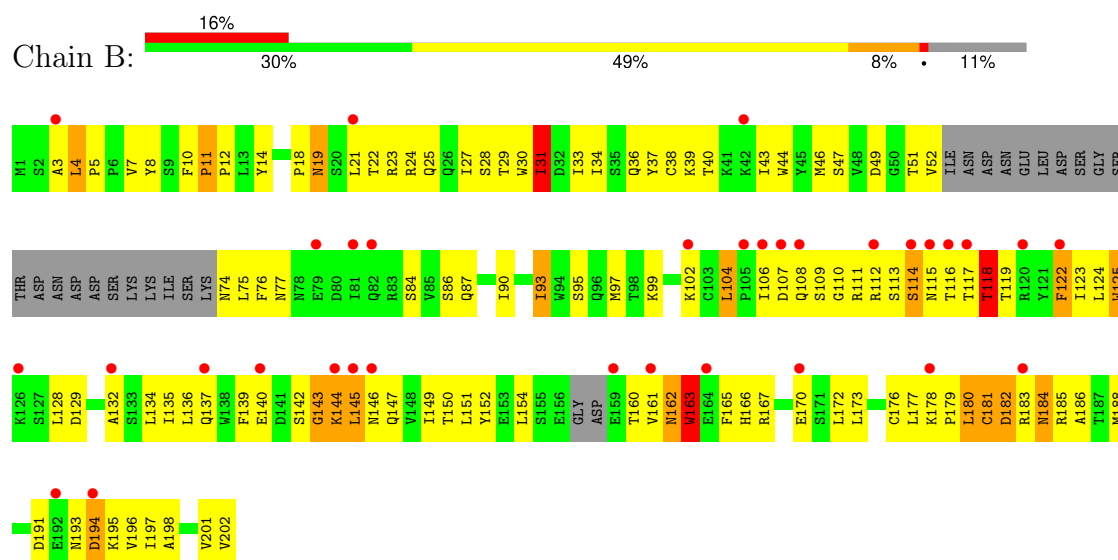
3 Residue-property plots

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: Hypothetical 23.6 kDa protein in YUH1-URA8 intergenic region



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.36Å 123.66Å 140.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 25.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-3.10) 93.5 (25.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 3.05Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.327 , 0.327 0.273 , 0.326	Depositor DCC
R_{free} test set	895 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5773	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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	0.59	0/1525	1.07	10/2066 (0.5%)
1	B	0.53	0/1516	1.07	16/2055 (0.8%)
1	C	0.58	0/1526	1.03	13/2070 (0.6%)
1	D	0.48	0/1321	1.06	12/1787 (0.7%)
All	All	0.55	0/5888	1.06	51/7978 (0.6%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	N-CA-C	-11.82	94.60	110.55
1	B	182	ASP	N-CA-C	-11.44	95.10	110.55
1	C	182	ASP	N-CA-C	-11.32	95.26	110.55
1	D	173	LEU	N-CA-C	-10.22	100.98	113.15
1	A	163	TRP	N-CA-C	-7.64	99.16	110.46
1	A	4	LEU	CA-C-N	7.20	127.80	120.38
1	A	4	LEU	C-N-CA	7.20	127.80	120.38
1	B	163	TRP	N-CA-C	-6.69	99.99	110.36
1	C	128	LEU	N-CA-C	-6.68	103.92	111.14
1	D	122	PHE	N-CA-C	-6.51	99.08	109.76
1	C	11	PRO	N-CA-C	6.31	118.40	110.70
1	B	104	LEU	CA-C-N	6.26	126.48	119.90
1	B	104	LEU	C-N-CA	6.26	126.48	119.90
1	C	163	TRP	N-CA-C	-6.24	100.68	110.36
1	B	10	PHE	CA-C-N	6.14	126.71	120.38
1	B	10	PHE	C-N-CA	6.14	126.71	120.38
1	A	10	PHE	CA-C-N	6.04	126.60	120.38
1	A	10	PHE	C-N-CA	6.04	126.60	120.38
1	D	26	GLN	N-CA-C	-6.04	104.76	111.71
1	A	11	PRO	N-CA-C	6.03	118.05	110.70
1	D	130	SER	N-CA-C	-6.00	101.74	111.04
1	D	148	VAL	N-CA-C	6.00	117.42	108.54
1	B	4	LEU	CA-C-N	5.92	126.48	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	C-N-CA	5.92	126.48	120.38
1	A	122	PHE	N-CA-C	-5.80	98.29	108.20
1	D	47	SER	CB-CA-C	-5.76	108.29	115.89
1	C	122	PHE	N-CA-C	-5.73	98.39	108.20
1	B	122	PHE	N-CA-C	-5.73	98.40	108.20
1	C	113	SER	N-CA-C	5.69	118.20	110.35
1	B	31	ILE	N-CA-C	-5.62	104.38	110.23
1	C	104	LEU	CA-C-N	5.62	125.80	119.90
1	C	104	LEU	C-N-CA	5.62	125.80	119.90
1	A	128	LEU	N-CA-C	-5.60	105.09	111.14
1	B	128	LEU	N-CA-C	-5.50	105.20	111.14
1	B	118	THR	N-CA-C	-5.48	100.86	109.25
1	D	4	LEU	CA-C-N	5.47	126.02	120.38
1	D	4	LEU	C-N-CA	5.47	126.02	120.38
1	B	11	PRO	N-CA-C	5.45	117.35	110.70
1	D	165	PHE	N-CA-C	-5.43	106.69	113.15
1	C	31	ILE	N-CA-C	-5.36	104.66	110.23
1	D	3	ALA	N-CA-C	-5.34	106.54	113.16
1	B	181	CYS	N-CA-C	-5.25	105.63	111.36
1	C	10	PHE	CA-C-N	5.22	125.75	120.38
1	C	10	PHE	C-N-CA	5.22	125.75	120.38
1	B	160	THR	N-CA-C	-5.11	107.43	113.97
1	C	120	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	118	THR	N-CA-C	-5.08	101.47	109.25
1	C	181	CYS	N-CA-C	-5.06	105.84	111.36
1	D	128	LEU	N-CA-C	-5.05	105.96	111.82
1	D	11	PRO	N-CA-C	5.04	116.85	110.70
1	B	93	ILE	CB-CA-C	-5.03	105.54	111.97

There are no chirality outliers.

There are no planarity outliers.

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	1492	0	1479	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1482	0	1468	127	0
1	C	1492	0	1474	141	0
1	D	1291	0	1290	177	0
2	A	5	0	0	1	0
2	B	2	0	0	0	0
2	C	7	0	0	1	0
2	D	2	0	0	1	0
All	All	5773	0	5711	550	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 50.

All (550) 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)
1:B:146:ASN:HA	1:B:202:VAL:HG22	1.35	1.07
1:C:104:LEU:HB3	1:C:122:PHE:HB3	1.45	0.97
1:D:37:TYR:HE1	1:D:41:LYS:HD2	1.31	0.95
1:C:74:ASN:ND2	1:C:76:PHE:H	1.66	0.93
1:C:115:ASN:C	1:C:117:THR:H	1.73	0.92
1:A:73:LYS:N	1:A:73:LYS:HZ2	1.67	0.91
1:D:128:LEU:HD12	1:D:128:LEU:H	1.36	0.89
1:B:150:THR:HA	1:B:198:ALA:HA	1.55	0.88
1:D:52:VAL:HG13	1:D:74:ASN:ND2	1.89	0.88
1:D:136:LEU:HB2	1:D:180:LEU:HD21	1.56	0.87
1:C:115:ASN:O	1:C:117:THR:N	2.07	0.87
1:A:112:ARG:O	1:A:118:THR:HB	1.76	0.85
1:B:145:LEU:O	1:B:202:VAL:HA	1.75	0.85
1:A:145:LEU:HD12	1:A:201:VAL:HG23	1.58	0.83
1:D:151:LEU:HB2	1:D:170:GLU:OE2	1.78	0.83
1:A:34:ILE:HG23	1:A:46:MET:HE2	1.62	0.81
1:D:154:LEU:HD12	1:D:173:LEU:HD21	1.63	0.81
1:B:115:ASN:O	1:B:117:THR:N	2.12	0.80
1:C:34:ILE:HG23	1:C:46:MET:HE2	1.64	0.79
1:C:18:PRO:O	1:C:19:ASN:HB2	1.83	0.79
1:B:34:ILE:HG23	1:B:46:MET:HE2	1.65	0.78
1:D:175:TYR:O	1:D:179:PRO:HD2	1.84	0.78
1:D:37:TYR:CE1	1:D:41:LYS:HD2	2.16	0.77
1:C:74:ASN:HD22	1:C:74:ASN:C	1.93	0.77
1:D:131:TRP:O	1:D:135:ILE:HG12	1.85	0.76
1:B:18:PRO:O	1:B:19:ASN:HB2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:O	1:A:19:ASN:HB2	1.84	0.76
1:C:176:CYS:O	1:C:179:PRO:HD2	1.87	0.75
1:B:43:ILE:HD13	1:B:52:VAL:HG12	1.67	0.75
1:C:74:ASN:HD22	1:C:75:LEU:N	1.85	0.75
1:B:95:SER:CB	1:C:193:ASN:HD22	2.01	0.74
1:D:150:THR:HA	1:D:198:ALA:HB2	1.70	0.74
1:B:150:THR:HG22	1:B:198:ALA:HB2	1.70	0.73
1:C:150:THR:HG22	1:C:198:ALA:HB2	1.71	0.73
1:B:95:SER:HB2	1:C:193:ASN:HD22	1.54	0.73
1:A:97:MET:HG3	1:A:102:LYS:HB2	1.71	0.72
1:D:122:PHE:CG	1:D:172:LEU:HD13	2.24	0.72
1:D:51:THR:HA	1:D:74:ASN:HB2	1.71	0.72
1:C:74:ASN:HD22	1:C:76:PHE:H	1.36	0.72
1:A:183:ARG:O	1:A:185:ARG:HG2	1.90	0.71
1:D:104:LEU:HD21	1:D:175:TYR:CE1	2.25	0.71
1:D:9:SER:O	1:D:11:PRO:HD3	1.90	0.71
1:D:27:ILE:HG23	1:D:93:ILE:HD13	1.71	0.71
1:D:172:LEU:C	1:D:174:TYR:H	1.98	0.71
1:A:80:ASP:HB3	1:C:116:THR:HG23	1.71	0.71
1:C:48:VAL:HG13	1:C:119:THR:O	1.90	0.71
1:C:122:PHE:CD2	1:C:172:LEU:HD13	2.26	0.71
1:A:11:PRO:HB2	1:A:12:PRO:HD3	1.72	0.71
1:C:151:LEU:HD11	1:C:196:VAL:HG12	1.72	0.70
1:D:149:ILE:O	1:D:198:ALA:HB1	1.91	0.70
1:C:31:ILE:HD13	1:C:97:MET:HB2	1.73	0.70
1:B:183:ARG:HH12	1:B:185:ARG:HG3	1.57	0.69
1:D:37:TYR:CE2	1:D:75:LEU:HD13	2.26	0.69
1:D:106:ILE:CD1	1:D:172:LEU:HD11	2.22	0.69
1:A:36:GLN:O	1:A:40:THR:HG23	1.91	0.69
1:D:37:TYR:HD2	1:D:75:LEU:HD22	1.58	0.69
1:D:106:ILE:HD13	1:D:172:LEU:HD21	1.75	0.69
1:B:99:LYS:HG3	1:C:195:LYS:HB2	1.76	0.68
1:A:42:LYS:HD2	2:A:205:HOH:O	1.92	0.68
1:D:23:ARG:O	1:D:27:ILE:HG13	1.93	0.68
1:B:31:ILE:HD13	1:B:97:MET:HB2	1.73	0.68
1:B:122:PHE:CD2	1:B:172:LEU:HD13	2.28	0.68
1:B:11:PRO:HB2	1:B:12:PRO:HD3	1.76	0.67
1:D:106:ILE:HD11	1:D:172:LEU:HD11	1.76	0.67
1:D:132:ALA:HB2	1:D:179:PRO:HG2	1.77	0.67
1:C:45:TYR:HB2	1:C:53:ILE:HB	1.77	0.67
1:A:122:PHE:CD2	1:A:172:LEU:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLN:HA	1:B:90:ILE:HD12	1.77	0.66
1:B:115:ASN:C	1:B:117:THR:H	2.03	0.66
1:D:87:GLN:HA	1:D:90:ILE:HD12	1.78	0.66
1:B:183:ARG:O	1:B:185:ARG:HG2	1.96	0.65
1:C:144:LYS:HA	1:C:147:GLN:OE1	1.96	0.65
1:A:53:ILE:HG21	1:A:120:ARG:NH2	2.11	0.65
1:B:162:ASN:H	1:B:163:TRP:HE3	1.44	0.65
1:D:138:TRP:CZ2	1:D:161:VAL:HG22	2.31	0.65
1:C:114:SER:HA	1:C:118:THR:CG2	2.27	0.65
1:A:30:TRP:O	1:A:34:ILE:HG12	1.97	0.65
1:B:186:ALA:HB2	1:B:201:VAL:HG12	1.79	0.64
1:B:129:ASP:O	1:B:132:ALA:HB3	1.97	0.64
1:A:183:ARG:HH12	1:A:185:ARG:HG3	1.60	0.64
1:C:183:ARG:O	1:C:185:ARG:HG2	1.96	0.64
1:D:52:VAL:HG13	1:D:74:ASN:HD22	1.62	0.64
1:D:175:TYR:O	1:D:178:LYS:HB2	1.97	0.64
1:B:30:TRP:O	1:B:34:ILE:HG12	1.98	0.64
1:B:182:ASP:O	1:B:183:ARG:HB2	1.98	0.64
1:C:36:GLN:O	1:C:40:THR:HG23	1.98	0.64
1:A:52:VAL:HG22	1:A:73:LYS:HB2	1.79	0.64
1:B:201:VAL:HG23	1:B:201:VAL:O	1.97	0.63
1:A:162:ASN:H	1:A:163:TRP:HE3	1.45	0.63
1:C:162:ASN:H	1:C:163:TRP:HE3	1.46	0.63
1:C:183:ARG:HH12	1:C:185:ARG:HG3	1.64	0.63
1:C:113:SER:N	1:C:116:THR:OG1	2.32	0.63
1:C:182:ASP:O	1:C:183:ARG:HB2	1.98	0.62
1:D:151:LEU:O	1:D:154:LEU:HB2	1.99	0.62
1:C:30:TRP:O	1:C:34:ILE:HG12	1.98	0.62
1:A:182:ASP:O	1:A:183:ARG:HB2	1.98	0.62
1:C:11:PRO:HB2	1:C:12:PRO:HD3	1.82	0.62
1:D:175:TYR:H	1:D:175:TYR:HD2	1.48	0.62
1:C:122:PHE:CE1	1:C:172:LEU:HB3	2.34	0.62
1:A:80:ASP:CB	1:C:116:THR:HG23	2.30	0.62
1:B:186:ALA:CB	1:B:201:VAL:HG12	2.29	0.61
1:B:114:SER:O	1:B:118:THR:HG22	2.00	0.61
1:D:139:PHE:HE1	1:D:149:ILE:HG21	1.65	0.61
1:C:32:ASP:CB	1:D:6:PRO:HG3	2.30	0.61
1:C:150:THR:HA	1:C:198:ALA:HA	1.82	0.61
1:D:147:GLN:HE22	1:D:149:ILE:HB	1.64	0.61
1:B:51:THR:HA	1:B:74:ASN:HB2	1.83	0.61
1:B:161:VAL:HG23	1:B:166:HIS:ND1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TRP:HE3	1:C:163:TRP:N	1.98	0.60
1:A:150:THR:HA	1:A:198:ALA:HA	1.84	0.60
1:A:181:CYS:SG	1:A:188:MET:HE2	2.41	0.60
1:A:31:ILE:HD13	1:A:97:MET:HB2	1.83	0.60
1:C:126:LYS:HB3	1:C:131:TRP:NE1	2.17	0.60
1:B:104:LEU:HB3	1:B:122:PHE:HB3	1.83	0.60
1:D:146:ASN:HA	1:D:201:VAL:O	2.01	0.60
1:D:150:THR:OG1	1:D:153:GLU:HB2	2.02	0.60
1:D:9:SER:HB3	1:D:81:ILE:HD11	1.83	0.59
1:C:144:LYS:NZ	1:C:160:THR:HG21	2.17	0.59
1:D:124:LEU:HD21	1:D:128:LEU:HG	1.84	0.59
1:A:97:MET:CG	1:A:102:LYS:HB2	2.32	0.59
1:D:46:MET:HA	1:D:53:ILE:HD12	1.83	0.59
1:A:122:PHE:CE1	1:A:172:LEU:HB3	2.37	0.59
1:B:36:GLN:O	1:B:40:THR:HG23	2.02	0.59
1:B:122:PHE:CE1	1:B:172:LEU:HB3	2.37	0.59
1:C:143:GLY:C	1:C:145:LEU:H	2.10	0.59
1:B:4:LEU:HD13	1:B:8:TYR:CE2	2.37	0.59
1:D:125:TRP:O	1:D:126:LYS:HB2	2.01	0.59
1:D:128:LEU:HD12	1:D:128:LEU:N	2.14	0.59
1:C:114:SER:HA	1:C:118:THR:HG22	1.85	0.59
1:D:135:ILE:O	1:D:138:TRP:HB3	2.03	0.59
1:B:3:ALA:HB1	1:B:37:TYR:CD2	2.38	0.58
1:B:134:LEU:HD11	1:B:163:TRP:HD1	1.68	0.58
1:B:163:TRP:HE3	1:B:163:TRP:N	2.01	0.58
1:C:186:ALA:HB2	1:C:201:VAL:HG12	1.84	0.58
1:D:138:TRP:HZ2	1:D:161:VAL:HG22	1.68	0.58
1:B:150:THR:HA	1:B:198:ALA:CA	2.32	0.58
1:B:143:GLY:C	1:B:145:LEU:H	2.12	0.58
1:B:107:ASP:C	1:B:109:SER:H	2.11	0.57
1:C:122:PHE:CZ	1:C:172:LEU:HB3	2.39	0.57
1:D:52:VAL:H	1:D:74:ASN:CB	2.17	0.57
1:D:122:PHE:CD1	1:D:172:LEU:HD22	2.39	0.57
1:A:143:GLY:C	1:A:145:LEU:H	2.13	0.56
1:D:174:TYR:CE1	1:D:188:MET:HE1	2.41	0.56
1:B:181:CYS:SG	1:B:188:MET:HE2	2.46	0.56
1:D:39:LYS:HG3	1:D:125:TRP:CE3	2.40	0.56
1:A:73:LYS:N	1:A:73:LYS:HD3	2.20	0.56
1:D:13:LEU:C	1:D:15:THR:H	2.14	0.56
1:D:175:TYR:N	1:D:175:TYR:CD2	2.73	0.56
1:B:122:PHE:CG	1:B:172:LEU:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HB3	1:A:179:PRO:HD3	1.87	0.56
1:B:19:ASN:HB3	1:B:22:THR:HB	1.87	0.55
1:A:25:GLN:HA	1:A:25:GLN:NE2	2.21	0.55
1:A:47:SER:OG	1:A:51:THR:HB	2.07	0.55
1:A:107:ASP:C	1:A:109:SER:H	2.12	0.55
1:D:16:ARG:CZ	1:D:23:ARG:NH1	2.69	0.55
1:C:26:GLN:HB2	1:D:10:PHE:HE1	1.72	0.55
1:C:32:ASP:CG	1:D:6:PRO:HG3	2.32	0.55
1:D:175:TYR:HD2	1:D:175:TYR:N	2.03	0.55
1:B:107:ASP:C	1:B:109:SER:N	2.63	0.55
1:D:106:ILE:CD1	1:D:172:LEU:HD21	2.37	0.55
1:D:154:LEU:CD1	1:D:173:LEU:HD21	2.36	0.55
1:B:150:THR:CG2	1:B:198:ALA:HB2	2.36	0.54
1:A:161:VAL:HG23	1:A:166:HIS:ND1	2.22	0.54
1:C:161:VAL:HG23	1:C:166:HIS:ND1	2.21	0.54
1:D:23:ARG:C	1:D:25:GLN:N	2.63	0.54
1:C:119:THR:HG23	1:C:120:ARG:HG2	1.90	0.54
1:A:3:ALA:H	1:A:40:THR:HG21	1.72	0.54
1:B:144:LYS:HA	1:B:147:GLN:OE1	2.07	0.54
1:C:19:ASN:HB3	1:C:22:THR:HB	1.89	0.54
1:D:46:MET:N	1:D:53:ILE:HD12	2.23	0.54
1:D:52:VAL:HG22	1:D:74:ASN:CG	2.32	0.54
1:D:106:ILE:HD11	1:D:122:PHE:HB2	1.90	0.54
1:A:145:LEU:O	1:A:145:LEU:HG	2.08	0.54
1:B:178:LYS:HB3	1:B:179:PRO:HD3	1.90	0.54
1:A:122:PHE:CG	1:A:172:LEU:HD13	2.43	0.54
1:A:163:TRP:HE3	1:A:163:TRP:N	2.05	0.54
1:D:5:PRO:HB2	1:D:7:VAL:HG13	1.89	0.54
1:A:129:ASP:O	1:A:132:ALA:HB3	2.07	0.54
1:C:126:LYS:HB3	1:C:131:TRP:CE2	2.43	0.54
1:C:191:ASP:OD2	1:C:191:ASP:C	2.52	0.53
1:A:30:TRP:O	1:A:31:ILE:C	2.52	0.53
1:C:135:ILE:HA	1:C:165:PHE:CE2	2.44	0.53
1:D:31:ILE:HG23	1:D:97:MET:HE3	1.89	0.53
1:D:22:THR:O	1:D:24:ARG:N	2.41	0.53
1:B:77:ASN:HA	1:B:84:SER:OG	2.08	0.53
1:C:34:ILE:CG2	1:C:46:MET:HE2	2.38	0.53
1:D:29:THR:O	1:D:33:ILE:HG13	2.08	0.53
1:D:122:PHE:CD1	1:D:172:LEU:HD13	2.44	0.53
1:B:3:ALA:HB1	1:B:37:TYR:CE2	2.44	0.53
1:B:107:ASP:O	1:B:109:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TYR:CB	1:C:53:ILE:HB	2.38	0.53
1:D:127:SER:OG	1:D:130:SER:HB2	2.09	0.53
1:B:47:SER:OG	1:B:51:THR:HB	2.09	0.53
1:B:102:LYS:O	1:B:124:LEU:HB2	2.08	0.53
1:C:25:GLN:HA	1:C:25:GLN:NE2	2.23	0.53
1:C:163:TRP:N	1:C:163:TRP:CE3	2.77	0.53
1:A:154:LEU:O	1:A:161:VAL:HG11	2.09	0.53
1:C:31:ILE:HG23	1:C:97:MET:HE3	1.91	0.53
1:C:106:ILE:HD11	1:C:120:ARG:HG3	1.90	0.53
1:D:53:ILE:HG22	1:D:53:ILE:O	2.08	0.53
1:C:181:CYS:SG	1:C:188:MET:HE2	2.49	0.53
1:A:4:LEU:HD22	1:A:8:TYR:CD2	2.44	0.52
1:A:19:ASN:HB3	1:A:22:THR:HB	1.90	0.52
1:A:45:TYR:HE1	1:A:106:ILE:CD1	2.21	0.52
1:C:106:ILE:HA	1:C:111:ARG:HA	1.91	0.52
1:D:52:VAL:CG1	1:D:74:ASN:ND2	2.66	0.52
1:D:34:ILE:HD13	1:D:75:LEU:HD23	1.91	0.52
1:D:124:LEU:C	1:D:126:LYS:H	2.17	0.52
1:D:134:LEU:O	1:D:135:ILE:C	2.52	0.52
1:D:161:VAL:O	1:D:166:HIS:ND1	2.29	0.52
1:A:9:SER:HA	1:A:81:ILE:HG13	1.91	0.52
1:D:150:THR:HA	1:D:198:ALA:CB	2.39	0.52
1:D:195:LYS:HG2	1:D:197:ILE:CD1	2.40	0.52
1:B:106:ILE:HG22	1:B:111:ARG:HA	1.91	0.52
1:C:140:GLU:C	1:C:142:SER:H	2.16	0.52
1:D:148:VAL:HG22	1:D:189:LEU:HD11	1.92	0.52
1:A:126:LYS:HB3	1:A:131:TRP:NE1	2.25	0.52
1:B:25:GLN:HA	1:B:25:GLN:NE2	2.24	0.52
1:D:23:ARG:HD2	1:D:89:PHE:CE2	2.45	0.52
1:D:30:TRP:HA	1:D:33:ILE:HD12	1.91	0.52
1:C:138:TRP:HD1	1:C:163:TRP:CE2	2.27	0.52
1:D:167:ARG:O	1:D:169:PRO:HD3	2.10	0.52
1:A:18:PRO:O	1:A:19:ASN:CB	2.55	0.51
1:B:112:ARG:O	1:B:118:THR:HB	2.10	0.51
1:A:153:GLU:O	1:A:158:ASP:N	2.43	0.51
1:C:152:TYR:CD1	1:C:152:TYR:C	2.88	0.51
1:A:73:LYS:N	1:A:73:LYS:CD	2.73	0.51
1:C:115:ASN:C	1:C:117:THR:N	2.47	0.51
1:C:129:ASP:O	1:C:132:ALA:HB3	2.11	0.51
1:C:145:LEU:O	1:C:145:LEU:HG	2.09	0.51
1:D:25:GLN:O	1:D:28:SER:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:TRP:HE3	1:D:122:PHE:HE2	1.57	0.51
1:D:51:THR:O	1:D:53:ILE:HG13	2.09	0.51
1:D:23:ARG:HA	1:D:26:GLN:HB2	1.92	0.51
1:B:140:GLU:C	1:B:142:SER:H	2.18	0.51
1:D:147:GLN:C	1:D:147:GLN:CD	2.78	0.51
1:A:14:TYR:N	1:A:14:TYR:CD2	2.79	0.51
1:A:144:LYS:HA	1:A:147:GLN:OE1	2.10	0.51
1:B:154:LEU:O	1:B:161:VAL:HG11	2.11	0.51
1:C:144:LYS:HZ1	1:C:160:THR:HG21	1.75	0.51
1:B:135:ILE:HA	1:B:165:PHE:CE2	2.46	0.51
1:D:131:TRP:HB3	1:D:176:CYS:HB3	1.93	0.51
1:D:192:GLU:O	1:D:192:GLU:HG3	2.11	0.51
1:B:176:CYS:O	1:B:179:PRO:HD2	2.10	0.50
1:D:190:LYS:HD3	1:D:194:ASP:HA	1.93	0.50
1:A:126:LYS:HB3	1:A:131:TRP:CE2	2.45	0.50
1:B:114:SER:HB3	1:C:192:GLU:OE2	2.12	0.50
1:A:140:GLU:C	1:A:142:SER:H	2.18	0.50
1:B:177:LEU:O	1:B:180:LEU:N	2.40	0.50
1:D:51:THR:O	1:D:52:VAL:C	2.55	0.50
1:A:9:SER:HB3	1:A:81:ILE:HD11	1.92	0.50
1:C:193:ASN:O	1:C:194:ASP:C	2.54	0.50
1:D:30:TRP:O	1:D:34:ILE:HG12	2.12	0.50
1:D:143:GLY:N	2:D:204:HOH:O	2.44	0.50
1:C:107:ASP:OD2	1:C:109:SER:N	2.45	0.50
1:D:136:LEU:HD22	1:D:180:LEU:CD2	2.42	0.50
1:B:163:TRP:N	1:B:163:TRP:CE3	2.79	0.50
1:A:25:GLN:HA	1:A:25:GLN:HE21	1.75	0.50
1:A:45:TYR:HA	1:A:121:TYR:O	2.12	0.50
1:A:80:ASP:HB3	1:C:116:THR:CG2	2.42	0.50
1:C:104:LEU:N	1:C:122:PHE:O	2.39	0.50
1:B:125:TRP:CD1	1:B:125:TRP:H	2.30	0.49
1:B:177:LEU:O	1:B:178:LYS:C	2.55	0.49
1:D:46:MET:HE2	1:D:50:GLY:HA2	1.94	0.49
1:D:46:MET:CA	1:D:53:ILE:HD12	2.43	0.49
1:D:154:LEU:HD12	1:D:173:LEU:CD2	2.39	0.49
1:A:73:LYS:N	1:A:73:LYS:NZ	2.51	0.49
1:A:185:ARG:HB3	1:A:185:ARG:NH1	2.27	0.49
1:B:177:LEU:O	1:B:180:LEU:HB2	2.13	0.49
1:A:104:LEU:HB3	1:A:122:PHE:HB3	1.94	0.49
1:B:30:TRP:O	1:B:31:ILE:C	2.55	0.49
1:C:166:HIS:O	1:C:167:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:CYS:C	1:C:179:PRO:HD2	2.37	0.49
1:D:131:TRP:HA	1:D:131:TRP:CE3	2.46	0.49
1:A:105:PRO:CB	1:A:113:SER:HB3	2.43	0.49
1:A:153:GLU:HG3	1:A:158:ASP:HB2	1.95	0.49
1:D:172:LEU:C	1:D:174:TYR:N	2.63	0.49
1:B:21:LEU:O	1:B:24:ARG:HB3	2.12	0.49
1:A:5:PRO:HD2	1:A:8:TYR:HB2	1.95	0.49
1:B:39:LYS:HG3	1:B:125:TRP:CE3	2.47	0.49
1:C:195:LYS:O	1:C:197:ILE:HG12	2.13	0.48
1:D:106:ILE:CD1	1:D:122:PHE:HB2	2.43	0.48
1:C:47:SER:OG	1:C:51:THR:HB	2.13	0.48
1:C:26:GLN:HB2	1:D:10:PHE:CE1	2.49	0.48
1:C:30:TRP:O	1:C:31:ILE:C	2.54	0.48
1:C:87:GLN:HA	1:C:90:ILE:HD12	1.95	0.48
1:D:183:ARG:O	1:D:184:ASN:C	2.56	0.48
1:B:95:SER:CB	1:C:193:ASN:ND2	2.73	0.48
1:C:131:TRP:O	1:C:135:ILE:HG13	2.14	0.48
1:D:37:TYR:CD2	1:D:75:LEU:HD22	2.44	0.48
1:D:199:ILE:HG12	1:D:200:LYS:N	2.27	0.48
1:B:19:ASN:H	1:B:23:ARG:NH2	2.11	0.48
1:B:179:PRO:O	1:B:182:ASP:O	2.32	0.48
1:C:18:PRO:O	1:C:19:ASN:CB	2.54	0.48
1:C:177:LEU:O	1:C:180:LEU:N	2.44	0.48
1:A:19:ASN:H	1:A:23:ARG:NH2	2.11	0.48
1:D:23:ARG:C	1:D:25:GLN:H	2.21	0.48
1:B:34:ILE:CG2	1:B:46:MET:HE2	2.38	0.47
1:C:154:LEU:O	1:C:161:VAL:HG11	2.14	0.47
1:D:181:CYS:O	1:D:182:ASP:C	2.57	0.47
1:B:107:ASP:C	1:B:119:THR:HG22	2.39	0.47
1:B:142:SER:C	1:B:144:LYS:H	2.22	0.47
1:D:37:TYR:HD2	1:D:75:LEU:CD2	2.25	0.47
1:D:38:CYS:CB	1:D:43:ILE:HB	2.44	0.47
1:D:136:LEU:HB2	1:D:180:LEU:CD2	2.36	0.47
1:D:148:VAL:CG2	1:D:189:LEU:HD11	2.44	0.47
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.28	0.47
1:B:166:HIS:O	1:B:167:ARG:HB2	2.13	0.47
1:C:168:MET:SD	1:C:173:LEU:HD13	2.55	0.47
1:A:190:LYS:HA	1:A:195:LYS:O	2.14	0.47
1:B:191:ASP:OD2	1:B:191:ASP:C	2.56	0.47
1:D:38:CYS:HB3	1:D:43:ILE:HB	1.95	0.47
1:C:14:TYR:N	1:C:14:TYR:CD2	2.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:TYR:CD1	1:D:121:TYR:N	2.82	0.47
1:D:174:TYR:HE1	1:D:188:MET:HE1	1.79	0.47
1:B:29:THR:O	1:B:33:ILE:HG13	2.15	0.47
1:C:140:GLU:HG2	1:C:145:LEU:HD22	1.96	0.47
1:A:38:CYS:SG	1:A:123:ILE:HG13	2.55	0.47
1:B:18:PRO:O	1:B:19:ASN:CB	2.55	0.47
1:C:25:GLN:HA	1:C:25:GLN:HE21	1.80	0.47
1:C:125:TRP:CD1	1:C:125:TRP:H	2.32	0.47
1:D:16:ARG:NH1	1:D:16:ARG:HG2	2.29	0.47
1:B:146:ASN:CA	1:B:202:VAL:HG22	2.23	0.47
1:D:175:TYR:O	1:D:179:PRO:CD	2.59	0.47
1:A:12:PRO:HB3	1:B:12:PRO:HB3	1.95	0.47
1:B:5:PRO:HD2	1:B:8:TYR:HB2	1.97	0.47
1:B:38:CYS:SG	1:B:123:ILE:HG13	2.54	0.47
1:D:16:ARG:NH2	1:D:23:ARG:HH22	2.13	0.47
1:C:10:PHE:CE1	1:D:26:GLN:HG3	2.50	0.47
1:C:142:SER:C	1:C:144:LYS:H	2.23	0.47
1:C:177:LEU:O	1:C:180:LEU:HB2	2.15	0.47
1:C:190:LYS:HE2	1:C:194:ASP:OD2	2.15	0.47
1:D:37:TYR:CD2	1:D:75:LEU:HD13	2.50	0.47
1:D:138:TRP:HD1	1:D:163:TRP:CE2	2.32	0.47
1:B:183:ARG:NH1	1:B:185:ARG:HG3	2.29	0.46
1:B:193:ASN:O	1:B:194:ASP:C	2.59	0.46
1:D:103:CYS:HA	1:D:124:LEU:H	1.79	0.46
1:A:5:PRO:HB2	1:A:7:VAL:HG12	1.98	0.46
1:A:155:SER:HB2	1:A:167:ARG:N	2.31	0.46
1:B:139:PHE:CD1	1:B:201:VAL:HG22	2.51	0.46
1:C:46:MET:HE3	1:C:94:TRP:CH2	2.51	0.46
1:A:87:GLN:HA	1:A:90:ILE:HD12	1.98	0.46
1:B:25:GLN:HA	1:B:25:GLN:HE21	1.80	0.46
1:B:31:ILE:HG23	1:B:97:MET:HE3	1.97	0.46
1:B:135:ILE:O	1:B:136:LEU:C	2.58	0.46
1:B:144:LYS:O	1:B:146:ASN:N	2.48	0.46
1:B:152:TYR:CD1	1:B:152:TYR:C	2.93	0.46
1:B:14:TYR:N	1:B:14:TYR:CD2	2.82	0.46
1:C:137:GLN:O	1:C:138:TRP:C	2.57	0.46
1:A:134:LEU:HD11	1:A:163:TRP:HD1	1.80	0.46
1:D:181:CYS:O	1:D:183:ARG:N	2.48	0.46
1:A:142:SER:C	1:A:144:LYS:H	2.24	0.46
1:D:17:GLN:HA	1:D:18:PRO:HD3	1.86	0.46
1:D:39:LYS:HG3	1:D:125:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ILE:O	1:D:81:ILE:HG22	2.16	0.46
1:D:89:PHE:O	1:D:92:GLU:N	2.49	0.46
1:C:185:ARG:HB3	1:C:185:ARG:NH1	2.31	0.46
1:A:4:LEU:HD22	1:A:8:TYR:CG	2.50	0.46
1:B:176:CYS:C	1:B:179:PRO:HD2	2.41	0.46
1:C:21:LEU:O	1:C:24:ARG:HB3	2.16	0.46
1:C:47:SER:OG	1:C:49:ASP:OD2	2.32	0.46
1:D:125:TRP:O	1:D:125:TRP:CE3	2.69	0.46
1:A:163:TRP:N	1:A:163:TRP:CE3	2.84	0.45
1:B:43:ILE:CD1	1:B:52:VAL:HG12	2.43	0.45
1:B:46:MET:SD	1:B:52:VAL:HG22	2.56	0.45
1:B:76:PHE:CE1	1:B:90:ILE:HG23	2.51	0.45
1:C:136:LEU:O	1:C:139:PHE:HB2	2.16	0.45
1:D:48:VAL:CG1	1:D:87:GLN:HE22	2.29	0.45
1:D:104:LEU:HB3	1:D:122:PHE:HB3	1.96	0.45
1:A:7:VAL:HG21	1:B:7:VAL:HG21	1.97	0.45
1:A:144:LYS:O	1:A:146:ASN:N	2.49	0.45
1:C:5:PRO:HD2	1:C:8:TYR:HB2	1.98	0.45
1:C:110:GLY:HA2	2:C:209:HOH:O	2.15	0.45
1:D:7:VAL:C	1:D:9:SER:H	2.22	0.45
1:C:151:LEU:HD11	1:C:196:VAL:CG1	2.45	0.45
1:D:4:LEU:HA	1:D:5:PRO:HD3	1.71	0.45
1:A:191:ASP:C	1:A:191:ASP:OD2	2.60	0.45
1:B:195:LYS:O	1:B:197:ILE:HG12	2.16	0.45
1:D:13:LEU:O	1:D:26:GLN:NE2	2.49	0.45
1:C:46:MET:HE3	1:C:94:TRP:HH2	1.81	0.45
1:D:22:THR:C	1:D:24:ARG:N	2.75	0.45
1:D:190:LYS:HA	1:D:195:LYS:O	2.16	0.45
1:A:23:ARG:O	1:A:27:ILE:HG13	2.17	0.45
1:C:81:ILE:HG22	1:C:81:ILE:O	2.16	0.45
1:C:90:ILE:O	1:C:93:ILE:HB	2.17	0.45
1:C:183:ARG:HB3	1:C:183:ARG:NH1	2.31	0.45
1:D:16:ARG:HG2	1:D:16:ARG:HH11	1.80	0.45
1:D:23:ARG:O	1:D:23:ARG:HG2	2.16	0.45
1:D:44:TRP:HE3	1:D:122:PHE:CE2	2.33	0.45
1:D:45:TYR:C	1:D:53:ILE:HD12	2.41	0.45
1:D:135:ILE:O	1:D:138:TRP:CB	2.64	0.45
1:D:164:GLU:C	1:D:166:HIS:H	2.23	0.45
1:A:140:GLU:HG2	1:A:145:LEU:HD22	1.97	0.45
1:B:43:ILE:CG2	1:B:44:TRP:N	2.80	0.45
1:C:134:LEU:HD11	1:C:163:TRP:HD1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:NH2	1:D:23:ARG:NH2	2.65	0.45
1:D:27:ILE:HG13	1:D:27:ILE:H	1.42	0.45
1:A:177:LEU:O	1:A:178:LYS:C	2.59	0.45
1:B:31:ILE:CD1	1:B:97:MET:HB2	2.44	0.45
1:B:51:THR:HA	1:B:74:ASN:CB	2.46	0.45
1:B:146:ASN:HA	1:B:202:VAL:CG2	2.26	0.45
1:C:144:LYS:C	1:C:146:ASN:H	2.25	0.45
1:A:152:TYR:CD1	1:A:152:TYR:C	2.94	0.45
1:D:104:LEU:HD21	1:D:175:TYR:CD1	2.52	0.45
1:A:89:PHE:O	1:A:92:GLU:N	2.50	0.44
1:B:102:LYS:C	1:B:124:LEU:HB2	2.42	0.44
1:C:144:LYS:O	1:C:146:ASN:N	2.51	0.44
1:D:48:VAL:HG12	1:D:87:GLN:HE22	1.83	0.44
1:D:77:ASN:HA	1:D:84:SER:OG	2.17	0.44
1:A:135:ILE:O	1:A:136:LEU:C	2.60	0.44
1:C:135:ILE:O	1:C:136:LEU:C	2.58	0.44
1:D:152:TYR:C	1:D:154:LEU:N	2.74	0.44
1:A:18:PRO:O	1:A:18:PRO:HG2	2.17	0.44
1:B:144:LYS:C	1:B:146:ASN:H	2.25	0.44
1:D:139:PHE:CE2	1:D:201:VAL:HG21	2.52	0.44
1:A:107:ASP:C	1:A:109:SER:N	2.76	0.44
1:A:154:LEU:HB3	1:A:173:LEU:HD21	2.00	0.44
1:B:52:VAL:HG21	1:B:75:LEU:HB2	2.00	0.44
1:C:143:GLY:C	1:C:145:LEU:N	2.75	0.44
1:C:177:LEU:O	1:C:178:LYS:C	2.60	0.44
1:D:130:SER:O	1:D:133:SER:N	2.50	0.44
1:A:193:ASN:O	1:A:194:ASP:C	2.61	0.44
1:B:4:LEU:HD13	1:B:8:TYR:CD2	2.52	0.44
1:C:5:PRO:HB2	1:C:7:VAL:HG12	1.99	0.44
1:A:89:PHE:O	1:A:90:ILE:C	2.60	0.44
1:A:177:LEU:O	1:A:180:LEU:HB2	2.18	0.44
1:A:182:ASP:O	1:A:183:ARG:CB	2.63	0.44
1:B:114:SER:HA	1:B:118:THR:HG21	2.00	0.44
1:C:179:PRO:O	1:C:182:ASP:O	2.35	0.44
1:A:81:ILE:O	1:A:81:ILE:HG22	2.18	0.44
1:D:130:SER:O	1:D:131:TRP:C	2.61	0.44
1:A:176:CYS:C	1:A:179:PRO:HD2	2.43	0.43
1:B:5:PRO:HB2	1:B:7:VAL:HG12	2.00	0.43
1:B:18:PRO:O	1:B:18:PRO:HG2	2.17	0.43
1:C:18:PRO:O	1:C:18:PRO:HG2	2.18	0.43
1:C:104:LEU:HD23	1:C:122:PHE:HD1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TRP:HD1	1:C:163:TRP:CZ2	2.36	0.43
1:C:182:ASP:O	1:C:183:ARG:CB	2.62	0.43
1:C:31:ILE:CG2	1:C:97:MET:HE3	2.48	0.43
1:D:28:SER:HA	1:D:31:ILE:HD12	1.98	0.43
1:A:4:LEU:HA	1:A:5:PRO:HD3	1.70	0.43
1:A:19:ASN:O	1:A:20:SER:C	2.61	0.43
1:C:94:TRP:O	1:C:95:SER:C	2.59	0.43
1:D:90:ILE:O	1:D:93:ILE:HB	2.18	0.43
1:C:76:PHE:CE1	1:C:90:ILE:HG23	2.53	0.43
1:A:138:TRP:HD1	1:A:163:TRP:CE2	2.37	0.43
1:D:128:LEU:H	1:D:128:LEU:CD1	2.05	0.43
1:C:4:LEU:HD13	1:C:8:TYR:CE2	2.53	0.43
1:D:177:LEU:HD13	1:D:199:ILE:HG21	2.00	0.43
1:A:144:LYS:C	1:A:146:ASN:H	2.27	0.43
1:A:166:HIS:O	1:A:167:ARG:HB2	2.19	0.43
1:C:111:ARG:HB3	1:C:175:TYR:OH	2.18	0.43
1:A:177:LEU:O	1:A:180:LEU:N	2.45	0.43
1:B:110:GLY:O	1:B:111:ARG:C	2.62	0.43
1:C:77:ASN:HA	1:C:84:SER:OG	2.19	0.43
1:C:113:SER:CA	1:C:116:THR:OG1	2.67	0.43
1:C:183:ARG:NH1	1:C:183:ARG:CB	2.81	0.43
1:D:14:TYR:CE1	1:D:30:TRP:HH2	2.36	0.43
1:D:51:THR:H	1:D:74:ASN:N	2.17	0.43
1:D:152:TYR:C	1:D:154:LEU:H	2.26	0.43
1:A:47:SER:OG	1:A:49:ASP:OD2	2.36	0.43
1:A:52:VAL:O	1:A:52:VAL:HG23	2.18	0.43
1:A:53:ILE:HG21	1:A:120:ARG:HH22	1.80	0.43
1:B:182:ASP:O	1:B:183:ARG:CB	2.63	0.43
1:C:52:VAL:HG22	1:C:73:LYS:O	2.18	0.43
1:C:154:LEU:HD12	1:C:154:LEU:HA	1.76	0.43
1:A:4:LEU:HG	1:A:37:TYR:HD2	1.82	0.42
1:A:45:TYR:CE1	1:A:106:ILE:HD11	2.54	0.42
1:A:90:ILE:O	1:A:93:ILE:HB	2.19	0.42
1:B:135:ILE:HG12	1:B:165:PHE:CD2	2.54	0.42
1:C:113:SER:OG	1:C:114:SER:N	2.52	0.42
1:C:199:ILE:HG12	1:C:200:LYS:N	2.34	0.42
1:D:14:TYR:CZ	1:D:78:ASN:HB2	2.54	0.42
1:D:124:LEU:C	1:D:126:LYS:N	2.77	0.42
1:A:137:GLN:O	1:A:138:TRP:C	2.62	0.42
1:A:183:ARG:NH1	1:A:183:ARG:CB	2.82	0.42
1:C:19:ASN:H	1:C:23:ARG:NH2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PHE:CG	1:C:172:LEU:HD13	2.55	0.42
1:A:122:PHE:CZ	1:A:172:LEU:HB3	2.54	0.42
1:D:177:LEU:CD1	1:D:199:ILE:HG21	2.49	0.42
1:A:113:SER:HA	1:A:118:THR:CG2	2.49	0.42
1:A:125:TRP:CD1	1:A:125:TRP:H	2.36	0.42
1:B:39:LYS:HA	1:B:125:TRP:CE2	2.54	0.42
1:B:149:ILE:HG12	1:B:150:THR:N	2.34	0.42
1:D:190:LYS:NZ	1:D:194:ASP:OD2	2.46	0.42
1:A:149:ILE:HG12	1:A:150:THR:N	2.33	0.42
1:C:87:GLN:O	1:C:88:VAL:C	2.62	0.42
1:A:17:GLN:HG2	1:A:26:GLN:OE1	2.20	0.42
1:B:86:SER:O	1:B:90:ILE:HG13	2.19	0.42
1:C:140:GLU:C	1:C:142:SER:N	2.78	0.42
1:C:153:GLU:C	1:C:155:SER:N	2.75	0.42
1:A:45:TYR:HE1	1:A:106:ILE:HD12	1.84	0.42
1:B:184:ASN:OD1	1:B:184:ASN:N	2.52	0.42
1:D:46:MET:HA	1:D:53:ILE:CD1	2.49	0.42
1:B:154:LEU:HB3	1:B:173:LEU:HD21	2.02	0.42
1:C:14:TYR:CE1	1:C:78:ASN:HB2	2.54	0.42
1:D:89:PHE:O	1:D:92:GLU:HB2	2.20	0.42
1:B:149:ILE:CG1	1:B:150:THR:N	2.82	0.42
1:B:152:TYR:HB2	1:B:170:GLU:OE1	2.19	0.42
1:D:52:VAL:H	1:D:74:ASN:HB3	1.84	0.42
1:B:28:SER:HA	1:B:31:ILE:HG13	2.02	0.41
1:B:90:ILE:O	1:B:93:ILE:HB	2.20	0.41
1:D:48:VAL:C	1:D:50:GLY:H	2.28	0.41
1:D:105:PRO:HA	1:D:121:TYR:CD2	2.54	0.41
1:D:176:CYS:O	1:D:179:PRO:HG2	2.19	0.41
1:A:11:PRO:C	1:A:13:LEU:N	2.78	0.41
1:A:45:TYR:HB3	1:A:53:ILE:HG13	2.01	0.41
1:B:140:GLU:C	1:B:142:SER:N	2.78	0.41
1:C:74:ASN:ND2	1:C:74:ASN:C	2.66	0.41
1:D:9:SER:HA	1:D:81:ILE:HG13	2.02	0.41
1:D:145:LEU:O	1:D:147:GLN:N	2.53	0.41
1:D:195:LYS:HG2	1:D:197:ILE:HD13	2.02	0.41
1:A:77:ASN:HA	1:A:84:SER:OG	2.20	0.41
1:C:143:GLY:O	1:C:145:LEU:N	2.52	0.41
1:B:122:PHE:CZ	1:B:172:LEU:HB3	2.56	0.41
1:D:178:LYS:O	1:D:181:CYS:N	2.38	0.41
1:A:25:GLN:HE21	1:A:25:GLN:CA	2.33	0.41
1:B:134:LEU:HD11	1:B:163:TRP:CD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:CZ	1:D:23:ARG:HH12	2.31	0.41
1:A:34:ILE:CG2	1:A:46:MET:HE2	2.42	0.41
1:A:48:VAL:HG13	1:A:119:THR:O	2.21	0.41
1:A:137:GLN:HE21	1:A:137:GLN:HB3	1.57	0.41
1:B:23:ARG:O	1:B:27:ILE:HG13	2.20	0.41
1:D:76:PHE:CE1	1:D:90:ILE:HG23	2.56	0.41
1:D:135:ILE:HD13	1:D:165:PHE:CG	2.56	0.41
1:A:143:GLY:C	1:A:145:LEU:N	2.78	0.41
1:B:142:SER:O	1:B:144:LYS:N	2.54	0.41
1:B:151:LEU:HD11	1:B:196:VAL:HG12	2.02	0.41
1:C:31:ILE:CD1	1:C:97:MET:HB2	2.46	0.41
1:C:94:TRP:O	1:C:98:THR:N	2.53	0.41
1:D:8:TYR:O	1:D:8:TYR:CG	2.74	0.41
1:D:13:LEU:HG	1:D:30:TRP:NE1	2.36	0.41
1:D:15:THR:HG22	1:D:16:ARG:O	2.21	0.41
1:D:41:LYS:O	1:D:43:ILE:N	2.54	0.41
1:D:191:ASP:OD1	1:D:191:ASP:C	2.63	0.41
1:C:178:LYS:HB3	1:C:179:PRO:HD3	2.03	0.41
1:C:11:PRO:HG2	1:D:22:THR:HG21	2.02	0.40
1:D:131:TRP:CZ3	1:D:134:LEU:HD23	2.55	0.40
1:D:131:TRP:HZ3	1:D:134:LEU:HD23	1.86	0.40
1:A:11:PRO:O	1:A:13:LEU:N	2.54	0.40
1:A:178:LYS:N	1:A:179:PRO:CD	2.84	0.40
1:B:49:ASP:C	1:B:49:ASP:OD2	2.64	0.40
1:A:139:PHE:CG	1:A:201:VAL:HG21	2.56	0.40
1:D:178:LYS:HB2	1:D:179:PRO:CD	2.51	0.40
1:D:178:LYS:O	1:D:179:PRO:C	2.64	0.40
1:C:142:SER:O	1:C:144:LYS:N	2.54	0.40
1:D:195:LYS:HG2	1:D:197:ILE:HD11	2.01	0.40
1:B:146:ASN:OD1	1:B:202:VAL:CG2	2.70	0.40
1:B:181:CYS:SG	1:B:188:MET:HG3	2.62	0.40
1:C:106:ILE:CG1	1:C:120:ARG:HG3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/202 (85%)	140 (81%)	23 (13%)	9 (5%)	1	10
1	B	173/202 (86%)	137 (79%)	25 (14%)	11 (6%)	1	6
1	C	174/202 (86%)	142 (82%)	22 (13%)	10 (6%)	1	8
1	D	140/202 (69%)	97 (69%)	30 (21%)	13 (9%)	0	3
All	All	659/808 (82%)	516 (78%)	100 (15%)	43 (6%)	1	6

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	109	SER
1	A	145	LEU
1	B	19	ASN
1	B	116	THR
1	B	145	LEU
1	C	19	ASN
1	C	116	THR
1	C	145	LEU
1	D	42	LYS
1	D	146	ASN
1	A	144	LYS
1	A	162	ASN
1	A	194	ASP
1	B	114	SER
1	B	144	LYS
1	B	194	ASP
1	C	144	LYS
1	C	194	ASP
1	D	23	ARG
1	D	46	MET
1	D	126	LYS
1	D	182	ASP
1	A	3	ALA
1	B	162	ASN
1	B	184	ASN
1	C	143	GLY
1	C	162	ASN

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Mol	Chain	Res	Type
1	D	51	THR
1	B	108	GLN
1	B	113	SER
1	B	143	GLY
1	C	114	SER
1	D	170	GLU
1	A	143	GLY
1	C	110	GLY
1	C	141	ASP
1	D	145	LEU
1	A	184	ASN
1	D	34	ILE
1	D	135	ILE
1	D	163	TRP
1	D	169	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	171/192 (89%)	161 (94%)	10 (6%)	18	48
1	B	170/192 (88%)	164 (96%)	6 (4%)	32	62
1	C	171/192 (89%)	164 (96%)	7 (4%)	27	59
1	D	148/192 (77%)	133 (90%)	15 (10%)	7	28
All	All	660/768 (86%)	622 (94%)	38 (6%)	18	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	53	ILE
1	A	73	LYS
1	A	109	SER
1	A	118	THR
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	125	TRP
1	A	137	GLN
1	A	163	TRP
1	A	180	LEU
1	B	31	ILE
1	B	118	THR
1	B	125	TRP
1	B	137	GLN
1	B	163	TRP
1	B	180	LEU
1	C	31	ILE
1	C	74	ASN
1	C	118	THR
1	C	125	TRP
1	C	137	GLN
1	C	163	TRP
1	C	180	LEU
1	D	7	VAL
1	D	15	THR
1	D	25	GLN
1	D	27	ILE
1	D	46	MET
1	D	52	VAL
1	D	121	TYR
1	D	124	LEU
1	D	128	LEU
1	D	161	VAL
1	D	167	ARG
1	D	175	TYR
1	D	184	ASN
1	D	187	THR
1	D	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	137	GLN
1	B	25	GLN
1	B	87	GLN
1	C	25	GLN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	96	GLN
1	C	137	GLN
1	C	193	ASN
1	D	25	GLN
1	D	74	ASN
1	D	87	GLN
1	D	147	GLN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	180/202 (89%)	0.62	18 (10%)	12 6	18, 42, 63, 79	30 (16%)
1	B	179/202 (88%)	1.15	33 (18%)	3 1	16, 48, 71, 81	43 (24%)
1	C	180/202 (89%)	0.71	19 (10%)	11 6	16, 43, 66, 80	37 (20%)
1	D	154/202 (76%)	1.00	23 (14%)	5 3	22, 57, 86, 104	26 (16%)
All	All	693/808 (85%)	0.86	93 (13%)	7 4	16, 46, 71, 104	136 (19%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	GLU	7.7
1	B	115	ASN	7.5
1	D	45	TYR	7.4
1	B	21	LEU	6.7
1	C	3	ALA	6.6
1	B	164	GLU	6.4
1	D	8	TYR	6.2
1	B	140	GLU	6.1
1	B	107	ASP	6.0
1	B	137	GLN	5.9
1	C	116	THR	5.9
1	B	79	GLU	5.9
1	B	159	GLU	5.5
1	D	183	ARG	5.3
1	A	116	THR	5.1
1	D	24	ARG	4.5
1	D	102	LYS	4.5
1	B	145	LEU	4.5
1	A	192	GLU	4.5
1	B	82	GLN	4.4
1	B	117	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	122	PHE	4.1
1	C	21	LEU	4.1
1	B	146	ASN	4.0
1	B	194	ASP	4.0
1	B	183	ARG	4.0
1	B	105	PRO	4.0
1	A	55	ASP	4.0
1	A	117	THR	4.0
1	A	21	LEU	3.9
1	D	164	GLU	3.9
1	A	112	ARG	3.9
1	D	79	GLU	3.9
1	D	42	LYS	3.6
1	A	164	GLU	3.6
1	B	42	LYS	3.5
1	C	163	TRP	3.5
1	B	108	GLN	3.3
1	C	79	GLU	3.2
1	C	112	ARG	3.2
1	C	117	THR	3.2
1	B	112	ARG	3.2
1	C	122	PHE	3.2
1	D	88	VAL	3.1
1	C	55	ASP	3.1
1	C	102	LYS	3.1
1	A	145	LEU	3.0
1	A	137	GLN	3.0
1	B	3	ALA	3.0
1	D	103	CYS	2.9
1	A	24	ARG	2.9
1	D	170	GLU	2.8
1	D	84	SER	2.8
1	B	192	GLU	2.8
1	C	44	TRP	2.8
1	B	106	ILE	2.8
1	D	122	PHE	2.8
1	B	126	LYS	2.8
1	A	146	ASN	2.7
1	B	116	THR	2.7
1	B	178	LYS	2.7
1	C	183	ARG	2.7
1	B	81	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	200	LYS	2.6
1	C	146	ASN	2.6
1	D	187	THR	2.6
1	A	79	GLU	2.5
1	B	102	LYS	2.5
1	D	153	GLU	2.5
1	D	83	ARG	2.5
1	B	170	GLU	2.5
1	B	120	ARG	2.5
1	D	75	LEU	2.5
1	C	96	GLN	2.5
1	A	43	ILE	2.4
1	A	162	ASN	2.4
1	D	91	ASP	2.4
1	C	39	LYS	2.3
1	C	148	VAL	2.3
1	B	132	ALA	2.3
1	A	40	THR	2.3
1	D	191	ASP	2.3
1	B	114	SER	2.2
1	A	167	ARG	2.2
1	C	108	GLN	2.2
1	A	141	ASP	2.2
1	B	161	VAL	2.2
1	D	146	ASN	2.1
1	D	3	ALA	2.1
1	C	45	TYR	2.1
1	A	108	GLN	2.0
1	B	144	LYS	2.0
1	D	154	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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.