



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:15 am BST

PDB ID : 4IDU
Title : crystal structure of Schmallenberg virus nucleoprotein
Authors : Dong, H.; Li, P.; Elliott, R.M.; Dong, C.
Deposited on : 2012-12-13
Resolution : 3.08 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

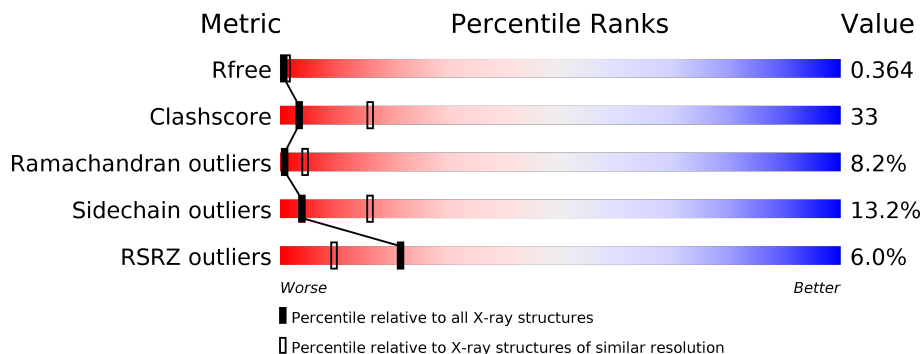
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 on 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	233	
1	C	233	
1	D	233	
2	B	233	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6838 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 SBV nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1714	1111	288	304	11	0	0	0
1	C	206	1635	1062	274	287	12	0	0	0
1	D	214	1704	1111	282	299	12	0	0	0

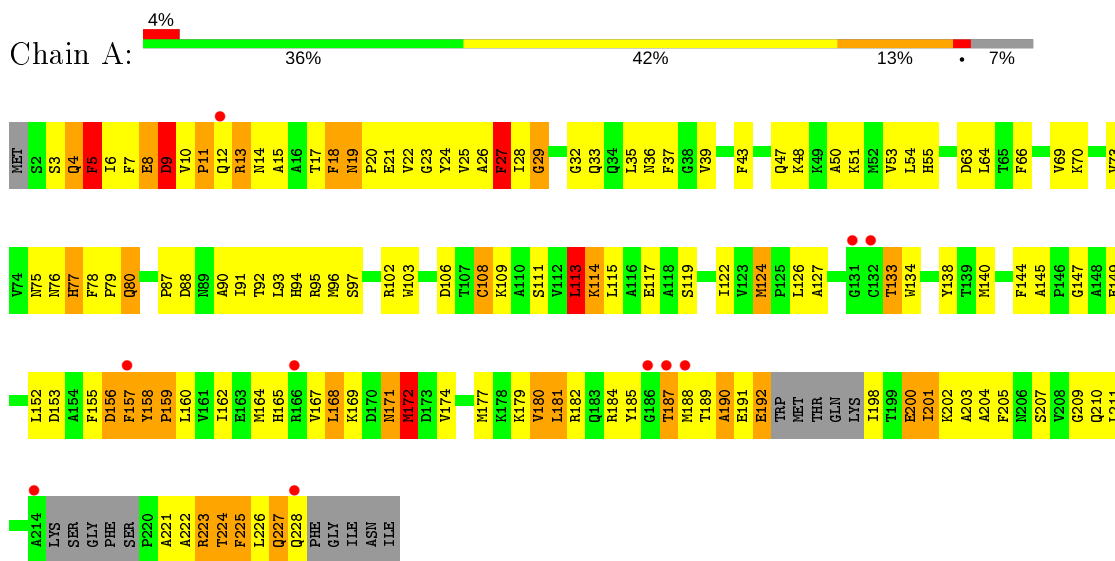
- Molecule 2 is a protein called SBV nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	225	1785	1159	300	314	10	2	0	0	0

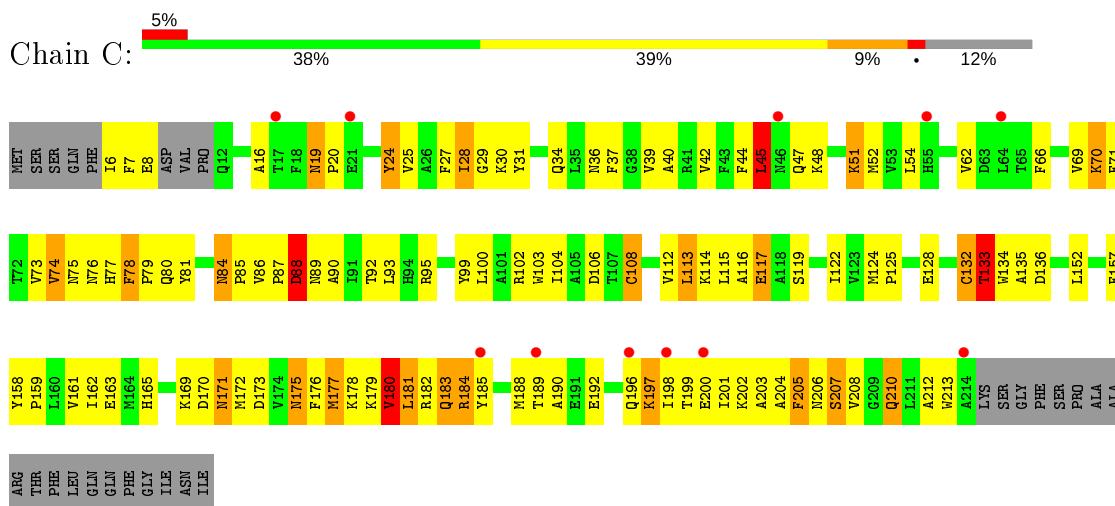
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA 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: SBV nucleoprotein

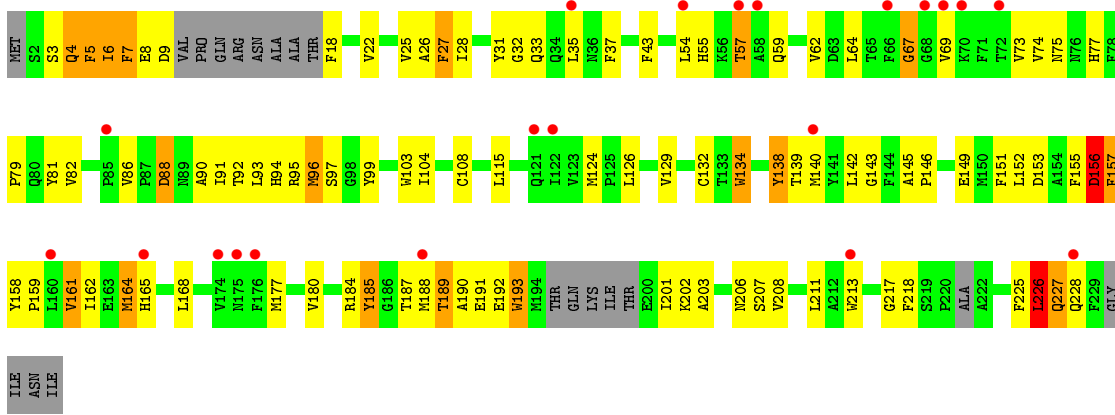


- Molecule 1: SBV nucleoprotein

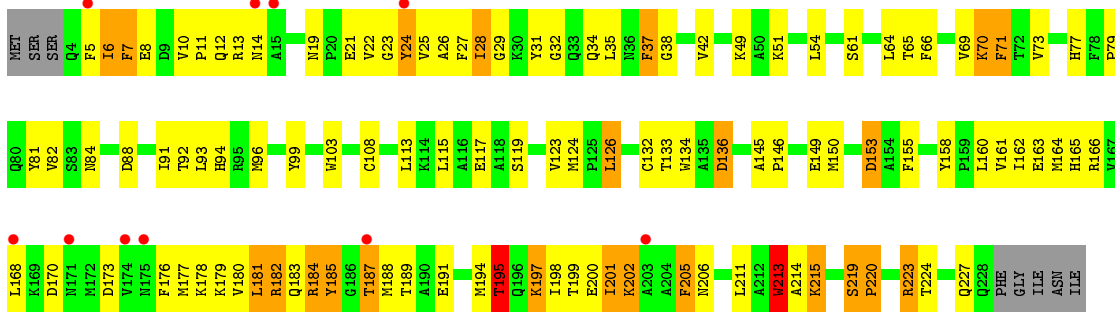


- Molecule 1: SBV nucleoprotein





• Molecule 2: SBV nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.32Å 86.44Å 77.40Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	29.71 – 3.08 33.92 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.71-3.08) 99.9 (33.92-3.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.06Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.321 , 0.364 0.320 , 0.364	Depositor DCC
R_{free} test set	960 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for l,-k,h	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6838	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.48	0/1756	0.71	3/2376 (0.1%)
1	C	0.56	1/1676 (0.1%)	0.70	3/2268 (0.1%)
1	D	0.51	4/1748 (0.2%)	0.65	2/2360 (0.1%)
2	B	0.56	1/1830 (0.1%)	0.81	7/2475 (0.3%)
All	All	0.53	6/7010 (0.1%)	0.72	15/9479 (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
2	B	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	TRP	CD2-CE2	5.35	1.47	1.41
1	C	213	TRP	CD2-CE2	5.34	1.47	1.41
1	D	134	TRP	CD2-CE2	5.18	1.47	1.41
1	D	213	TRP	CD2-CE2	5.11	1.47	1.41
2	B	213	TRP	CD2-CE2	5.08	1.47	1.41
1	D	193	TRP	CD2-CE2	5.02	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	TYR	N-CA-C	-9.49	85.37	111.00
2	B	28	ILE	N-CA-C	-7.10	91.84	111.00
2	B	195	THR	N-CA-C	6.43	128.37	111.00
1	A	172	MET	N-CA-C	-6.39	93.75	111.00
1	C	180	VAL	N-CA-CB	6.16	125.05	111.50
2	B	185	TYR	N-CA-CB	5.96	121.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	LYS	N-CA-C	5.92	126.98	111.00
1	C	45	LEU	N-CA-C	-5.58	95.94	111.00
1	C	45	LEU	CA-CB-CG	5.34	127.58	115.30
2	B	71	PHE	N-CA-C	5.25	125.16	111.00
2	B	202	LYS	N-CA-C	5.23	125.12	111.00
1	A	113	LEU	CA-CB-CG	5.18	127.21	115.30
1	D	156	ASP	N-CA-C	5.16	124.93	111.00
2	B	28	ILE	N-CA-CB	5.12	122.58	110.80
1	A	225	PHE	CB-CA-C	5.11	120.62	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	GLY	Peptide
2	B	69	VAL	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	1714	0	1699	143	0
1	C	1635	0	1626	132	0
1	D	1704	0	1677	75	0
2	B	1785	0	1772	96	0
All	All	6838	0	6774	443	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 33.

All (443) 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:202:LYS:O	2:B:205:PHE:CD1	1.65	1.50
1:C:161:VAL:HG21	1:C:203:ALA:CB	1.54	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:CE2	1:A:102:ARG:HD3	1.58	1.37
1:A:190:ALA:CB	1:A:191:GLU:HA	1.65	1.26
1:A:27:PHE:HE2	1:A:102:ARG:CD	1.54	1.20
1:C:161:VAL:HG21	1:C:203:ALA:HB3	1.18	1.18
1:A:190:ALA:HB1	1:A:192:GLU:N	1.61	1.13
2:B:202:LYS:O	2:B:205:PHE:HD1	1.01	1.12
1:A:190:ALA:HB1	1:A:192:GLU:H	1.07	1.11
1:A:190:ALA:HB3	1:A:191:GLU:HA	1.11	1.10
1:A:12:GLN:HA	1:A:13:ARG:HB2	1.32	1.09
1:A:167:VAL:HB	1:A:172:MET:HB3	1.25	1.08
2:B:187:THR:HG22	2:B:188:MET:H	1.22	1.03
1:A:190:ALA:CB	1:A:191:GLU:CA	2.38	1.01
1:C:84:ASN:HB3	1:C:85:PRO:HD3	1.38	1.01
2:B:165:HIS:CE1	2:B:205:PHE:O	2.17	0.96
1:C:161:VAL:HG21	1:C:203:ALA:HB1	1.47	0.96
1:A:27:PHE:HE2	1:A:102:ARG:HD3	0.95	0.95
2:B:219:SER:HB2	2:B:220:PRO:HD2	1.49	0.95
2:B:21:GLU:O	2:B:24:TYR:HB3	1.67	0.93
1:C:132:CYS:O	1:C:133:THR:HB	1.68	0.93
1:C:192:GLU:O	1:C:196:GLN:HB2	1.68	0.93
1:C:84:ASN:HB3	1:C:85:PRO:CD	1.98	0.93
1:C:161:VAL:CG2	1:C:203:ALA:CB	2.45	0.93
2:B:219:SER:HB2	2:B:220:PRO:CD	1.99	0.92
1:A:12:GLN:HA	1:A:13:ARG:CB	2.01	0.90
2:B:27:PHE:HB2	2:B:32:GLY:HA3	1.53	0.90
1:C:76:ASN:HD21	1:C:86:VAL:CG2	1.84	0.90
1:C:196:GLN:CG	1:C:200:GLU:HG3	2.04	0.88
1:A:27:PHE:O	1:A:29:GLY:N	2.05	0.88
1:A:167:VAL:CB	1:A:172:MET:HB3	2.07	0.85
1:C:74:VAL:HG11	1:C:90:ALA:HB1	1.59	0.84
2:B:27:PHE:CB	2:B:32:GLY:HA3	2.07	0.84
1:C:161:VAL:CG2	1:C:203:ALA:HB3	2.07	0.83
1:C:196:GLN:CD	1:C:200:GLU:HG3	1.99	0.83
1:A:20:PRO:HA	1:A:24:TYR:HE2	1.42	0.82
1:C:196:GLN:HG2	1:C:200:GLU:CG	2.13	0.79
1:C:70:LYS:HD3	1:C:70:LYS:H	1.47	0.79
1:A:157:PHE:CE1	1:A:200:GLU:HB3	2.17	0.79
1:D:4:GLN:HE21	1:D:4:GLN:HA	1.48	0.79
1:C:184:ARG:NH1	1:C:192:GLU:HG3	1.99	0.78
2:B:73:VAL:HG22	2:B:96:MSE:HE1	1.65	0.77
1:C:44:PHE:O	1:C:45:LEU:HB3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HA	1:A:24:TYR:CE2	2.19	0.77
1:D:129:VAL:O	1:D:217:GLY:HA3	1.84	0.77
1:A:158:TYR:O	1:A:162:ILE:HG12	1.85	0.76
1:A:190:ALA:HB1	1:A:191:GLU:CA	2.12	0.76
1:A:164:MET:O	1:A:168:LEU:HB2	1.86	0.76
2:B:6:ILE:HG13	2:B:7:PHE:H	1.50	0.75
2:B:194:MET:HG3	2:B:195:THR:HG23	1.68	0.75
1:A:190:ALA:HB1	1:A:191:GLU:HA	1.66	0.75
1:A:12:GLN:CA	1:A:13:ARG:HB2	2.14	0.74
1:C:203:ALA:HA	1:C:207:SER:HB3	1.68	0.74
1:C:161:VAL:CG2	1:C:203:ALA:HB1	2.13	0.74
1:C:196:GLN:HG2	1:C:200:GLU:HG2	1.70	0.74
1:C:54:LEU:HD11	1:C:62:VAL:HG21	1.70	0.73
1:D:156:ASP:O	1:D:157:PHE:HB2	1.88	0.73
1:C:159:PRO:O	1:C:163:GLU:HG2	1.87	0.73
1:A:152:LEU:HD21	1:A:157:PHE:HB3	1.70	0.73
1:C:184:ARG:HH12	1:C:192:GLU:HG3	1.54	0.73
1:C:157:PHE:HE1	1:C:184:ARG:HD3	1.54	0.73
1:A:184:ARG:HB3	1:A:188:MET:HE3	1.69	0.73
1:A:158:TYR:H	1:A:159:PRO:HD3	1.54	0.73
1:A:198:ILE:HD12	1:A:201:ILE:HB	1.69	0.72
1:C:34:GLN:HB3	1:C:69:VAL:HG11	1.72	0.72
1:A:190:ALA:CB	1:A:192:GLU:H	1.95	0.71
1:A:108:CYS:SG	1:A:115:LEU:HD22	2.30	0.71
1:A:124:MET:SD	1:A:145:ALA:HB2	2.30	0.71
1:A:153:ASP:HB3	1:A:185:TYR:HA	1.73	0.70
1:A:19:ASN:HB3	1:A:20:PRO:HD3	1.74	0.70
1:C:192:GLU:O	1:C:196:GLN:CB	2.39	0.70
1:A:201:ILE:O	1:A:204:ALA:N	2.22	0.70
1:A:167:VAL:HB	1:A:172:MET:CB	2.14	0.69
1:A:200:GLU:HG3	1:A:203:ALA:HB3	1.73	0.69
2:B:8:GLU:HG3	2:B:179:LYS:NZ	2.07	0.69
1:D:3:SER:HB2	1:D:4:GLN:HA	1.75	0.68
1:A:15:ALA:HB3	1:A:18:PHE:CD2	2.28	0.68
2:B:187:THR:CG2	2:B:188:MET:H	2.02	0.68
2:B:187:THR:HG22	2:B:188:MET:HG2	1.75	0.68
1:C:88:ASP:O	1:C:90:ALA:N	2.27	0.68
1:C:203:ALA:O	1:C:207:SER:HB3	1.92	0.68
2:B:187:THR:HG22	2:B:188:MET:N	2.04	0.67
2:B:91:ILE:HG12	2:B:96:MSE:HB2	1.76	0.67
2:B:219:SER:CB	2:B:220:PRO:CD	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HG	1:A:157:PHE:HA	1.76	0.67
1:A:15:ALA:HB3	1:A:18:PHE:CE2	2.30	0.67
2:B:22:VAL:HG12	2:B:99:TYR:OH	1.94	0.66
1:C:77:HIS:O	1:C:78:PHE:HB3	1.96	0.66
1:A:184:ARG:HB3	1:A:188:MET:CE	2.25	0.66
1:C:165:HIS:CE1	1:C:204:ALA:HA	2.31	0.66
1:A:27:PHE:CE2	1:A:102:ARG:CD	2.40	0.66
2:B:155:PHE:O	2:B:158:TYR:HD1	1.77	0.66
1:C:183:GLN:HG2	1:C:184:ARG:H	1.60	0.66
1:D:64:LEU:HD12	1:D:73:VAL:HG21	1.76	0.66
1:D:27:PHE:O	1:D:32:GLY:N	2.29	0.66
1:D:153:ASP:HB3	1:D:185:TYR:HA	1.77	0.66
1:C:196:GLN:HG2	1:C:200:GLU:HG3	1.77	0.65
2:B:25:VAL:O	2:B:29:GLY:HA3	1.96	0.65
1:C:20:PRO:HA	1:C:24:TYR:HD1	1.60	0.65
1:A:11:PRO:HB2	1:A:13:ARG:HH12	1.62	0.65
2:B:6:ILE:HG22	2:B:176:PHE:CZ	2.32	0.65
1:A:19:ASN:HB3	1:A:20:PRO:CD	2.28	0.64
2:B:223:ARG:HD2	2:B:223:ARG:N	2.13	0.64
2:B:38:GLY:O	2:B:42:VAL:HG23	1.98	0.64
1:C:178:LYS:HD3	1:C:182:ARG:HH21	1.63	0.64
1:A:190:ALA:HB1	1:A:191:GLU:C	2.16	0.64
1:C:202:LYS:O	1:C:206:ASN:HB3	1.98	0.64
2:B:92:THR:HG22	2:B:94:HIS:H	1.63	0.63
1:D:59:GLN:HE21	1:D:62:VAL:HG13	1.62	0.63
1:A:167:VAL:HA	1:A:171:ASN:O	1.97	0.63
1:C:201:ILE:O	1:C:205:PHE:N	2.23	0.63
1:C:165:HIS:O	1:C:169:LYS:N	2.27	0.63
2:B:6:ILE:CG2	2:B:176:PHE:CZ	2.82	0.62
1:C:180:VAL:O	1:C:182:ARG:N	2.30	0.62
1:C:87:PRO:O	1:C:90:ALA:HB3	1.98	0.62
1:C:19:ASN:HB3	1:C:20:PRO:CD	2.29	0.62
1:D:54:LEU:HG	1:D:75:ASN:ND2	2.14	0.62
1:D:140:MET:HB3	1:D:211:LEU:HD11	1.82	0.62
1:C:198:ILE:O	1:C:202:LYS:HB2	1.99	0.62
1:D:104:ILE:HD11	1:D:142:LEU:HD21	1.81	0.62
1:C:161:VAL:O	1:C:165:HIS:ND1	2.31	0.62
1:A:222:ALA:HB2	2:B:181:LEU:HD22	1.82	0.61
2:B:32:GLY:HA2	2:B:35:LEU:HD12	1.81	0.61
2:B:162:ILE:O	2:B:166:ARG:HG2	2.01	0.61
1:A:171:ASN:O	1:A:172:MET:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:CB	1:C:69:VAL:HG11	2.30	0.61
1:A:23:GLY:O	1:A:27:PHE:HB2	2.01	0.61
1:C:208:VAL:HG12	1:C:208:VAL:O	2.00	0.61
1:C:74:VAL:HG22	1:C:92:THR:HG22	1.80	0.61
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.83	0.61
1:C:184:ARG:HB3	1:C:190:ALA:HA	1.83	0.61
1:D:92:THR:HG22	1:D:95:ARG:HD2	1.83	0.61
2:B:181:LEU:O	2:B:182:ARG:HB2	2.01	0.61
2:B:223:ARG:HG3	2:B:227:GLN:HG3	1.83	0.60
1:A:9:ASP:O	1:A:10:VAL:HB	2.00	0.60
1:A:189:THR:O	1:A:190:ALA:HB2	2.00	0.60
1:A:158:TYR:N	1:A:159:PRO:HD3	2.15	0.60
1:A:158:TYR:N	1:A:159:PRO:CD	2.64	0.60
1:A:27:PHE:CZ	1:A:102:ARG:HD3	2.30	0.60
1:A:200:GLU:O	1:A:201:ILE:C	2.40	0.60
1:C:84:ASN:CB	1:C:85:PRO:CD	2.78	0.60
1:C:48:LYS:HG3	1:C:51:LYS:HE3	1.84	0.60
1:C:196:GLN:CG	1:C:200:GLU:CG	2.72	0.60
1:C:70:LYS:HD3	1:C:70:LYS:N	2.14	0.60
1:C:48:LYS:O	1:C:52:MET:HG3	2.02	0.60
1:D:185:TYR:HB3	1:D:190:ALA:HB2	1.85	0.59
1:C:197:LYS:O	1:C:201:ILE:HG12	2.03	0.58
1:A:27:PHE:HE2	1:A:102:ARG:HD2	1.60	0.58
1:D:161:VAL:HG21	1:D:208:VAL:HB	1.85	0.58
1:C:177:MET:O	1:C:180:VAL:HG22	2.03	0.58
1:D:59:GLN:HG3	1:D:62:VAL:HG22	1.86	0.57
1:C:76:ASN:HD21	1:C:86:VAL:HG22	1.64	0.57
2:B:6:ILE:HG13	2:B:7:PHE:N	2.18	0.57
1:C:203:ALA:CA	1:C:207:SER:HB3	2.34	0.57
2:B:51:LYS:HG3	2:B:77:HIS:CE1	2.39	0.57
1:C:180:VAL:C	1:C:182:ARG:H	2.08	0.57
1:C:36:ASN:HA	1:C:103:TRP:HH2	1.70	0.56
2:B:64:LEU:HB3	2:B:66:PHE:CE1	2.40	0.56
2:B:65:THR:HG23	2:B:70:LYS:H	1.70	0.56
1:A:37:PHE:CD1	1:A:103:TRP:HZ3	2.23	0.56
2:B:198:ILE:HB	2:B:201:ILE:HB	1.88	0.56
2:B:91:ILE:HD11	2:B:96:MSE:HA	1.88	0.56
1:D:140:MET:CB	1:D:211:LEU:HD11	2.36	0.56
1:A:22:VAL:O	1:A:25:VAL:HG12	2.06	0.55
1:A:7:PHE:HD1	1:A:8:GLU:N	2.04	0.55
1:A:39:VAL:HG11	1:A:69:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:HIS:HD2	1:A:77:HIS:O	1.89	0.55
2:B:119:SER:HA	2:B:134:TRP:CE2	2.42	0.55
1:A:19:ASN:O	1:A:21:GLU:N	2.40	0.55
1:C:183:GLN:H	1:C:183:GLN:CD	2.10	0.55
1:C:199:THR:O	1:C:202:LYS:HB3	2.07	0.55
2:B:8:GLU:HG3	2:B:179:LYS:HZ3	1.71	0.55
1:D:31:TYR:O	1:D:35:LEU:HB2	2.06	0.55
1:A:8:GLU:O	1:A:9:ASP:HB2	2.08	0.54
2:B:219:SER:CB	2:B:220:PRO:HD2	2.30	0.54
1:A:17:THR:O	1:A:19:ASN:N	2.41	0.54
1:A:226:LEU:O	1:A:228:GLN:HG3	2.06	0.54
1:A:158:TYR:O	1:A:162:ILE:CG1	2.53	0.54
2:B:223:ARG:HG3	2:B:223:ARG:HH11	1.73	0.54
1:C:192:GLU:O	1:C:196:GLN:CG	2.55	0.54
1:D:6:ILE:HG23	1:D:7:PHE:HB2	1.89	0.54
2:B:37:PHE:CD1	2:B:103:TRP:HZ3	2.25	0.54
1:C:203:ALA:C	1:C:207:SER:HB3	2.28	0.54
1:A:79:PRO:O	1:A:80:GLN:HG3	2.08	0.54
2:B:181:LEU:O	2:B:182:ARG:CB	2.56	0.54
1:C:197:LYS:CG	1:C:198:ILE:H	2.21	0.54
1:C:54:LEU:HG	1:C:75:ASN:CG	2.29	0.53
1:A:32:GLY:HA2	1:A:35:LEU:HD22	1.91	0.53
1:C:69:VAL:HG23	1:C:71:PHE:CZ	2.43	0.53
1:D:158:TYR:HE1	1:D:207:SER:HB2	1.74	0.53
1:A:156:ASP:O	1:A:158:TYR:N	2.41	0.53
1:D:104:ILE:CD1	1:D:142:LEU:HD21	2.39	0.53
1:D:138:TYR:CE2	1:D:139:THR:HG23	2.43	0.53
1:C:6:ILE:O	1:C:7:PHE:HB3	2.08	0.53
2:B:64:LEU:HB3	2:B:66:PHE:HE1	1.73	0.53
2:B:8:GLU:HG3	2:B:179:LYS:HZ1	1.72	0.53
1:C:76:ASN:ND2	1:C:86:VAL:CG2	2.64	0.53
1:A:140:MET:HE1	1:A:211:LEU:HD11	1.89	0.53
1:C:183:GLN:HG2	1:C:184:ARG:N	2.24	0.53
1:D:164:MET:O	1:D:168:LEU:N	2.36	0.53
1:D:3:SER:H	1:D:4:GLN:HE21	1.56	0.53
1:C:165:HIS:O	1:C:169:LYS:HG2	2.08	0.52
1:D:225:PHE:O	1:D:227:GLN:N	2.38	0.52
1:C:179:LYS:O	1:C:180:VAL:HG13	2.08	0.52
1:C:114:LYS:HA	1:C:117:GLU:HG2	1.90	0.52
1:C:19:ASN:HB3	1:C:20:PRO:HD3	1.91	0.52
2:B:161:VAL:HA	2:B:164:MET:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG13	1:A:88:ASP:O	2.09	0.52
1:A:93:LEU:HA	1:A:96:MET:HE3	1.91	0.52
1:A:177:MET:O	1:A:180:VAL:HG23	2.10	0.52
2:B:124:MET:CE	2:B:145:ALA:HB2	2.40	0.52
2:B:6:ILE:HG21	2:B:176:PHE:HZ	1.74	0.52
1:C:119:SER:HA	1:C:134:TRP:CE2	2.45	0.52
1:D:74:VAL:HG11	1:D:90:ALA:HB1	1.92	0.51
2:B:32:GLY:C	2:B:34:GLN:H	2.13	0.51
2:B:31:TYR:O	2:B:35:LEU:HG	2.11	0.51
2:B:79:PRO:HA	2:B:82:VAL:HG23	1.92	0.51
1:C:76:ASN:HA	1:C:81:TYR:O	2.09	0.51
1:D:5:PHE:HD2	1:D:6:ILE:HG13	1.75	0.51
1:A:157:PHE:CE1	1:A:200:GLU:CB	2.91	0.51
1:C:181:LEU:HD23	1:C:184:ARG:HH22	1.76	0.51
1:A:153:ASP:HB3	1:A:185:TYR:CA	2.39	0.51
1:C:180:VAL:HG23	1:C:181:LEU:N	2.26	0.51
2:B:126:LEU:HD13	2:B:146:PRO:HD3	1.92	0.51
1:C:170:ASP:O	1:C:171:ASN:HB2	2.11	0.51
1:D:152:LEU:HD23	1:D:159:PRO:HG2	1.92	0.51
1:D:59:GLN:NE2	1:D:62:VAL:HG13	2.25	0.51
1:A:140:MET:HE3	1:A:211:LEU:HD21	1.91	0.51
1:C:152:LEU:HD23	1:C:157:PHE:HD1	1.75	0.51
2:B:197:LYS:O	2:B:201:ILE:HG22	2.11	0.51
1:A:200:GLU:O	1:A:202:LYS:N	2.44	0.50
1:D:185:TYR:H	1:D:190:ALA:HB3	1.76	0.50
1:D:158:TYR:O	1:D:162:ILE:HG12	2.11	0.50
2:B:150:MSE:HA	2:B:183:GLN:HG2	1.94	0.50
1:D:108:CYS:SG	1:D:115:LEU:HA	2.52	0.50
1:D:140:MET:SD	1:D:211:LEU:HD21	2.52	0.50
1:D:22:VAL:O	1:D:25:VAL:HG22	2.11	0.50
1:D:59:GLN:HG3	1:D:59:GLN:O	2.11	0.50
1:C:88:ASP:C	1:C:90:ALA:H	2.15	0.50
1:D:54:LEU:HD22	1:D:93:LEU:HD12	1.94	0.49
1:A:179:LYS:HG3	1:A:182:ARG:HH21	1.77	0.49
1:A:224:THR:O	1:A:224:THR:OG1	2.29	0.49
2:B:6:ILE:HG21	2:B:176:PHE:CZ	2.47	0.49
1:A:223:ARG:CZ	2:B:177:MET:SD	3.00	0.49
2:B:5:PHE:CB	2:B:7:PHE:CZ	2.96	0.49
1:D:156:ASP:O	1:D:157:PHE:CB	2.59	0.49
1:A:48:LYS:NZ	1:A:126:LEU:HG	2.26	0.49
1:A:54:LEU:HD11	1:A:64:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:HA	1:A:117:GLU:OE2	2.12	0.49
1:C:54:LEU:HD11	1:C:62:VAL:CG2	2.42	0.49
1:A:7:PHE:CD1	1:A:8:GLU:N	2.81	0.49
1:C:87:PRO:O	1:C:90:ALA:CB	2.61	0.49
2:B:94:HIS:HE1	2:B:149:GLU:OE2	1.95	0.49
1:D:99:TYR:CE1	1:D:151:PHE:HZ	2.31	0.49
1:C:177:MET:O	1:C:178:LYS:C	2.50	0.49
1:C:181:LEU:HD23	1:C:184:ARG:NH2	2.28	0.49
1:A:25:VAL:HG13	1:A:26:ALA:N	2.27	0.49
1:D:27:PHE:O	1:D:32:GLY:CA	2.61	0.49
2:B:12:GLN:C	2:B:14:ASN:H	2.15	0.48
1:A:207:SER:HA	1:A:210:GLN:HE21	1.78	0.48
1:A:55:HIS:CD2	1:A:79:PRO:HD3	2.48	0.48
2:B:187:THR:O	2:B:191:GLU:HG3	2.13	0.48
2:B:205:PHE:CG	2:B:206:ASN:N	2.81	0.48
1:C:152:LEU:HD23	1:C:157:PHE:CD1	2.49	0.48
2:B:165:HIS:NE2	2:B:205:PHE:O	2.46	0.48
2:B:22:VAL:O	2:B:22:VAL:HG12	2.14	0.48
1:C:178:LYS:CD	1:C:182:ARG:HH21	2.25	0.48
2:B:19:ASN:OD1	2:B:150:MSE:HB3	2.13	0.48
1:C:112:VAL:O	1:C:115:LEU:HB3	2.13	0.48
1:C:183:GLN:O	1:C:184:ARG:O	2.32	0.48
1:A:111:SER:HB2	1:A:113:LEU:HD13	1.95	0.48
1:D:140:MET:CG	1:D:211:LEU:HD11	2.44	0.48
1:A:102:ARG:NH1	1:A:106:ASP:OD2	2.47	0.48
1:D:139:THR:HG22	1:D:155:PHE:HD1	1.79	0.48
2:B:136:ASP:OD1	2:B:136:ASP:N	2.47	0.47
1:C:178:LYS:HD3	1:C:182:ARG:NH2	2.28	0.47
1:A:190:ALA:HB3	1:A:191:GLU:CA	2.05	0.47
2:B:194:MET:O	2:B:195:THR:OG1	2.29	0.47
1:C:19:ASN:CB	1:C:20:PRO:CD	2.92	0.47
1:D:124:MET:SD	1:D:145:ALA:HB2	2.54	0.47
1:D:91:ILE:O	1:D:91:ILE:HG12	2.14	0.47
2:B:214:ALA:O	2:B:215:LYS:C	2.52	0.47
1:C:113:LEU:O	1:C:116:ALA:N	2.48	0.47
1:D:184:ARG:HB3	1:D:187:THR:HA	1.96	0.47
1:D:27:PHE:N	1:D:27:PHE:CD1	2.81	0.47
1:A:19:ASN:C	1:A:21:GLU:H	2.17	0.47
2:B:73:VAL:HG22	2:B:96:MSE:CE	2.39	0.47
2:B:81:TYR:HB3	2:B:84:ASN:HD22	1.79	0.47
1:D:134:TRP:HZ3	1:D:138:TYR:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:SER:CB	1:D:4:GLN:HA	2.37	0.47
1:C:28:ILE:HG23	1:C:29:GLY:N	2.30	0.47
1:A:43:PHE:HE2	1:A:97:SER:HB3	1.79	0.47
1:C:188:MET:HG2	1:C:189:THR:HG23	1.97	0.47
1:A:37:PHE:HD1	1:A:103:TRP:HZ3	1.61	0.47
1:C:134:TRP:C	1:C:136:ASP:H	2.17	0.47
1:C:203:ALA:O	1:C:207:SER:CB	2.63	0.47
1:A:75:ASN:HD21	1:A:78:PHE:HB2	1.79	0.47
1:C:27:PHE:HD2	1:C:102:ARG:HH22	1.61	0.47
1:A:10:VAL:CG1	1:A:11:PRO:HD2	2.43	0.46
1:D:226:LEU:O	1:D:227:GLN:CB	2.63	0.46
1:A:11:PRO:HB2	1:A:13:ARG:NH1	2.28	0.46
1:D:165:HIS:HA	1:D:168:LEU:HB2	1.95	0.46
1:D:5:PHE:CD2	1:D:6:ILE:HG13	2.50	0.46
1:A:96:MET:HB2	1:A:96:MET:HE2	1.79	0.46
1:A:127:ALA:HB2	1:A:144:PHE:HB2	1.97	0.46
1:C:28:ILE:HG23	1:C:29:GLY:H	1.80	0.46
1:D:92:THR:HG21	1:D:95:ARG:HH11	1.79	0.46
2:B:202:LYS:O	2:B:205:PHE:CE1	2.52	0.46
1:A:18:PHE:HE1	1:A:95:ARG:HH12	1.63	0.46
1:A:18:PHE:HD1	1:A:22:VAL:HG11	1.81	0.46
1:C:158:TYR:HA	1:C:161:VAL:HG22	1.97	0.46
2:B:22:VAL:CG2	2:B:88:ASP:O	2.64	0.46
1:C:158:TYR:O	1:C:159:PRO:C	2.53	0.46
1:C:158:TYR:O	1:C:162:ILE:HG12	2.16	0.46
2:B:22:VAL:CG1	2:B:88:ASP:O	2.64	0.45
1:A:226:LEU:O	1:A:227:GLN:C	2.55	0.45
1:A:94:HIS:NE2	1:A:147:GLY:HA2	2.32	0.45
1:D:27:PHE:O	1:D:32:GLY:HA3	2.17	0.45
1:C:44:PHE:CE2	1:C:100:LEU:HB3	2.52	0.45
1:D:67:GLY:C	1:D:69:VAL:H	2.20	0.45
1:D:184:ARG:HG3	1:D:191:GLU:HB2	1.97	0.45
1:A:165:HIS:CD2	1:A:169:LYS:HD2	2.51	0.45
1:A:171:ASN:O	1:A:172:MET:CB	2.64	0.45
1:C:210:GLN:O	1:C:210:GLN:HG3	2.17	0.45
1:A:37:PHE:CE1	1:A:103:TRP:CZ3	3.04	0.45
1:A:4:GLN:HA	1:A:4:GLN:HE21	1.82	0.45
1:A:5:PHE:CD1	1:A:5:PHE:C	2.90	0.45
1:D:25:VAL:O	1:D:27:PHE:N	2.50	0.45
1:A:19:ASN:CB	1:A:20:PRO:CD	2.94	0.45
1:A:64:LEU:HB3	1:A:66:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PHE:O	1:C:73:VAL:HG23	2.17	0.45
1:D:3:SER:N	1:D:4:GLN:HE21	2.15	0.45
1:D:79:PRO:HA	1:D:82:VAL:HG23	1.98	0.45
1:C:88:ASP:C	1:C:90:ALA:N	2.68	0.45
1:D:27:PHE:N	1:D:27:PHE:HD1	2.15	0.45
1:A:13:ARG:HB2	1:A:13:ARG:CZ	2.47	0.45
2:B:108:CYS:HB2	2:B:115:LEU:HA	1.99	0.45
1:C:196:GLN:CD	1:C:200:GLU:CG	2.81	0.45
1:C:114:LYS:HA	1:C:117:GLU:CG	2.47	0.44
1:C:173:ASP:HB3	1:C:176:PHE:CE1	2.52	0.44
1:A:189:THR:O	1:A:190:ALA:CB	2.66	0.44
2:B:155:PHE:O	2:B:158:TYR:CD1	2.65	0.44
2:B:213:TRP:CD1	2:B:214:ALA:N	2.85	0.44
1:C:180:VAL:C	1:C:182:ARG:N	2.70	0.44
1:C:70:LYS:CD	1:C:70:LYS:H	2.23	0.44
1:D:126:LEU:HD12	1:D:126:LEU:H	1.83	0.44
1:D:3:SER:H	1:D:4:GLN:HB2	1.82	0.44
1:A:5:PHE:HD2	1:A:92:THR:HG21	1.83	0.44
1:A:92:THR:HG22	1:A:95:ARG:HD2	1.99	0.44
1:D:3:SER:H	1:D:4:GLN:NE2	2.16	0.44
1:A:177:MET:O	1:A:181:LEU:HD13	2.17	0.44
1:A:73:VAL:HG13	1:A:91:ILE:O	2.17	0.44
1:C:95:ARG:HB3	1:C:99:TYR:CE2	2.52	0.44
1:D:153:ASP:HA	1:D:185:TYR:CD2	2.52	0.44
1:A:157:PHE:CZ	1:A:200:GLU:HB3	2.50	0.44
1:A:153:ASP:N	1:A:153:ASP:OD1	2.42	0.44
1:A:18:PHE:CD1	1:A:22:VAL:HG11	2.52	0.44
1:A:3:SER:OG	1:A:51:LYS:HE3	2.18	0.44
2:B:199:THR:O	2:B:200:GLU:HG2	2.17	0.44
2:B:202:LYS:C	2:B:205:PHE:CD1	2.72	0.44
1:D:161:VAL:O	1:D:164:MET:HB2	2.17	0.44
1:A:37:PHE:HB3	1:A:122:ILE:HD11	1.99	0.44
1:C:81:TYR:HA	1:C:84:ASN:ND2	2.33	0.43
1:A:124:MET:SD	1:A:145:ALA:CB	3.04	0.43
1:A:3:SER:HB2	1:A:77:HIS:ND1	2.33	0.43
2:B:25:VAL:HG23	2:B:26:ALA:N	2.32	0.43
2:B:92:THR:HG22	2:B:94:HIS:N	2.31	0.43
1:C:77:HIS:O	1:C:78:PHE:CB	2.66	0.43
1:C:44:PHE:HE2	1:C:100:LEU:HB3	1.82	0.43
1:C:188:MET:HA	1:C:189:THR:HA	1.70	0.43
1:C:31:TYR:OH	1:C:71:PHE:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ALA:HB1	1:C:104:ILE:HD11	2.01	0.43
1:C:157:PHE:CE1	1:C:184:ARG:HD3	2.43	0.43
1:D:203:ALA:HA	1:D:206:ASN:OD1	2.18	0.43
1:A:152:LEU:CD2	1:A:157:PHE:HB3	2.44	0.43
1:D:189:THR:CG2	1:D:202:LYS:HD2	2.48	0.43
1:A:4:GLN:O	1:A:5:PHE:CB	2.66	0.43
2:B:153:ASP:HA	2:B:185:TYR:CD2	2.54	0.43
1:C:124:MET:HA	1:C:125:PRO:HD3	1.88	0.43
1:D:185:TYR:C	1:D:185:TYR:CD1	2.92	0.43
2:B:132:CYS:HA	2:B:211:LEU:HD11	2.00	0.43
1:C:7:PHE:CG	1:C:8:GLU:N	2.86	0.43
1:A:92:THR:O	1:A:95:ARG:HB2	2.19	0.43
1:D:104:ILE:HD11	1:D:142:LEU:HD11	2.01	0.42
2:B:163:GLU:OE1	2:B:166:ARG:NE	2.52	0.42
2:B:223:ARG:CD	2:B:223:ARG:N	2.74	0.42
2:B:27:PHE:CB	2:B:32:GLY:CA	2.89	0.42
1:A:39:VAL:HG13	1:A:66:PHE:O	2.19	0.42
1:D:91:ILE:HD11	1:D:96:MET:HE3	1.99	0.42
1:C:7:PHE:CD2	1:C:8:GLU:N	2.87	0.42
1:D:149:GLU:HG3	1:D:180:VAL:HG12	2.00	0.42
1:A:48:LYS:HZ3	1:A:126:LEU:HG	1.85	0.42
1:C:30:LYS:HE3	1:C:31:TYR:CZ	2.55	0.42
1:D:59:GLN:CG	1:D:62:VAL:HG22	2.49	0.42
2:B:178:LYS:C	2:B:182:ARG:HH21	2.22	0.42
1:D:94:HIS:CD2	1:D:146:PRO:HB2	2.54	0.42
2:B:27:PHE:O	2:B:27:PHE:CD1	2.73	0.42
2:B:177:MET:C	2:B:179:LYS:N	2.70	0.42
1:C:175:ASN:OD1	1:C:175:ASN:N	2.50	0.42
1:D:177:MET:O	1:D:180:VAL:HG22	2.20	0.42
1:D:192:GLU:O	1:D:193:TRP:HB3	2.20	0.42
1:A:205:PHE:O	1:A:209:GLY:N	2.53	0.42
2:B:133:THR:HG22	2:B:134:TRP:H	1.83	0.42
1:C:100:LEU:O	1:C:104:ILE:HD12	2.20	0.42
1:C:208:VAL:CG1	1:C:208:VAL:O	2.67	0.42
1:C:108:CYS:HB3	1:C:115:LEU:HA	2.01	0.41
1:C:47:GLN:O	1:C:51:LYS:HB3	2.20	0.41
2:B:160:LEU:C	2:B:160:LEU:HD23	2.41	0.41
1:A:9:ASP:O	1:A:10:VAL:CB	2.65	0.41
1:A:109:LYS:HE3	1:A:138:TYR:HE1	1.86	0.41
1:A:23:GLY:O	1:A:27:PHE:HD2	2.03	0.41
1:A:50:ALA:HA	1:A:53:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:VAL:HG23	1:C:181:LEU:HG	2.02	0.41
1:C:27:PHE:O	1:C:29:GLY:N	2.54	0.41
1:D:8:GLU:CD	1:D:9:ASP:H	2.23	0.41
1:A:140:MET:CE	1:A:211:LEU:HD11	2.50	0.41
1:A:64:LEU:HD23	1:A:66:PHE:HZ	1.85	0.41
2:B:124:MET:HE1	2:B:145:ALA:HB2	2.03	0.41
2:B:37:PHE:CD1	2:B:103:TRP:CZ3	3.07	0.41
1:A:119:SER:HA	1:A:134:TRP:CD1	2.56	0.41
1:A:37:PHE:CD1	1:A:103:TRP:CZ3	3.07	0.41
1:A:47:GLN:HE22	1:A:97:SER:HB3	1.86	0.41
2:B:32:GLY:HA2	2:B:35:LEU:CD1	2.49	0.41
1:C:180:VAL:HG23	1:C:181:LEU:H	1.85	0.41
1:C:37:PHE:HB3	1:C:122:ILE:HD11	2.03	0.41
1:A:167:VAL:HG21	1:A:174:VAL:HG22	2.03	0.40
1:A:4:GLN:CA	1:A:4:GLN:HE21	2.33	0.40
1:C:39:VAL:HG22	1:C:66:PHE:O	2.22	0.40
1:C:31:TYR:CZ	1:C:71:PHE:HA	2.56	0.40
1:A:222:ALA:HB2	2:B:181:LEU:CD2	2.51	0.40
1:A:43:PHE:CE2	1:A:97:SER:HB3	2.57	0.40
2:B:160:LEU:HA	2:B:180:VAL:HG11	2.03	0.40
1:D:18:PHE:HB3	1:D:88:ASP:OD2	2.21	0.40
1:A:165:HIS:NE2	1:A:169:LYS:HD2	2.36	0.40
1:A:23:GLY:O	1:A:27:PHE:CD2	2.74	0.40
1:A:87:PRO:HB2	1:A:90:ALA:H	1.86	0.40
2:B:205:PHE:CD1	2:B:206:ASN:N	2.84	0.40
1:C:133:THR:HG23	1:C:135:ALA:H	1.86	0.40
1:A:119:SER:HA	1:A:134:TRP:CG	2.56	0.40
1:C:39:VAL:O	1:C:42:VAL:HG12	2.22	0.40
1:D:43:PHE:CE2	1:D:97:SER:HA	2.57	0.40
1:A:54:LEU:HB3	1:A:77:HIS:CD2	2.57	0.40
2:B:92:THR:CG2	2:B:93:LEU:N	2.85	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	211/233 (91%)	152 (72%)	32 (15%)	27 (13%)	0	1
1	C	202/233 (87%)	134 (66%)	52 (26%)	16 (8%)	1	5
1	D	206/233 (88%)	149 (72%)	47 (23%)	10 (5%)	2	12
2	B	223/233 (96%)	158 (71%)	49 (22%)	16 (7%)	1	5
All	All	842/932 (90%)	593 (70%)	180 (21%)	69 (8%)	1	4

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	9	ASP
1	A	11	PRO
1	A	13	ARG
1	A	18	PHE
1	A	19	ASN
1	A	80	GLN
1	A	157	PHE
1	A	172	MET
1	A	190	ALA
2	B	24	TYR
2	B	28	ILE
2	B	182	ARG
2	B	184	ARG
2	B	219	SER
1	C	19	ASN
1	C	28	ILE
1	C	45	LEU
1	C	84	ASN
1	C	88	ASP
1	C	133	THR
1	C	180	VAL
1	C	184	ARG
1	D	156	ASP
1	D	157	PHE
1	D	188	MET
1	D	226	LEU
1	A	8	GLU
1	A	28	ILE
1	A	29	GLY

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Mol	Chain	Res	Type
1	A	200	GLU
1	A	201	ILE
1	A	227	GLN
2	B	187	THR
1	C	16	ALA
1	C	89	ASN
1	C	132	CYS
1	C	171	ASN
1	C	181	LEU
1	C	212	ALA
1	D	227	GLN
1	A	27	PHE
1	A	133	THR
2	B	7	PHE
2	B	195	THR
1	C	79	PRO
1	D	67	GLY
1	A	171	ASN
1	A	225	PHE
2	B	6	ILE
2	B	11	PRO
2	B	37	PHE
2	B	215	LYS
1	C	78	PHE
1	D	57	THR
1	A	14	ASN
1	A	187	THR
1	A	221	ALA
1	A	223	ARG
2	B	71	PHE
2	B	170	ASP
1	D	6	ILE
1	D	143	GLY
1	A	156	ASP
2	B	13	ARG
2	B	220	PRO
1	D	26	ALA
1	A	158	TYR
1	A	159	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/193 (93%)	154 (86%)	25 (14%)	3	14
1	C	170/193 (88%)	146 (86%)	24 (14%)	3	14
1	D	178/193 (92%)	154 (86%)	24 (14%)	4	15
2	B	186/191 (97%)	165 (89%)	21 (11%)	6	22
All	All	713/770 (93%)	619 (87%)	94 (13%)	4	16

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	PHE
1	A	6	ILE
1	A	9	ASP
1	A	27	PHE
1	A	33	GLN
1	A	36	ASN
1	A	63	ASP
1	A	70	LYS
1	A	76	ASN
1	A	77	HIS
1	A	108	CYS
1	A	113	LEU
1	A	114	LYS
1	A	124	MET
1	A	133	THR
1	A	149	GLU
1	A	155	PHE
1	A	160	LEU
1	A	168	LEU
1	A	180	VAL
1	A	181	LEU
1	A	187	THR
1	A	192	GLU

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Mol	Chain	Res	Type
1	A	224	THR
2	B	10	VAL
2	B	49	LYS
2	B	54	LEU
2	B	61	SER
2	B	113	LEU
2	B	117	GLU
2	B	123	VAL
2	B	126	LEU
2	B	136	ASP
2	B	153	ASP
2	B	168	LEU
2	B	173	ASP
2	B	181	LEU
2	B	184	ARG
2	B	189	THR
2	B	197	LYS
2	B	201	ILE
2	B	205	PHE
2	B	213	TRP
2	B	223	ARG
2	B	224	THR
1	C	24	TYR
1	C	25	VAL
1	C	45	LEU
1	C	51	LYS
1	C	70	LYS
1	C	74	VAL
1	C	80	GLN
1	C	88	ASP
1	C	93	LEU
1	C	106	ASP
1	C	108	CYS
1	C	113	LEU
1	C	117	GLU
1	C	128	GLU
1	C	133	THR
1	C	172	MET
1	C	175	ASN
1	C	177	MET
1	C	183	GLN
1	C	185	TYR

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Mol	Chain	Res	Type
1	C	197	LYS
1	C	205	PHE
1	C	207	SER
1	C	210	GLN
1	D	4	GLN
1	D	5	PHE
1	D	7	PHE
1	D	27	PHE
1	D	28	ILE
1	D	33	GLN
1	D	37	PHE
1	D	55	HIS
1	D	57	THR
1	D	77	HIS
1	D	81	TYR
1	D	86	VAL
1	D	88	ASP
1	D	96	MET
1	D	132	CYS
1	D	156	ASP
1	D	161	VAL
1	D	164	MET
1	D	185	TYR
1	D	189	THR
1	D	201	ILE
1	D	218	PHE
1	D	226	LEU
1	D	228	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	33	GLN
1	A	47	GLN
1	A	55	HIS
1	A	210	GLN
2	B	12	GLN
2	B	19	ASN
2	B	46	ASN
2	B	77	HIS
2	B	94	HIS

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Mol	Chain	Res	Type
2	B	121	GLN
2	B	183	GLN
2	B	196	GLN
1	C	76	ASN
1	C	84	ASN
1	C	171	ASN
1	D	4	GLN
1	D	59	GLN
1	D	89	ASN
1	D	94	HIS
1	D	121	GLN
1	D	183	GLN
1	D	228	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	217/233 (93%)	0.23	10 (4%) 32 15	59, 102, 145, 195	0
1	C	206/233 (88%)	0.05	11 (5%) 26 12	43, 86, 119, 136	0
1	D	214/233 (91%)	0.40	21 (9%) 7 2	72, 116, 161, 175	0
2	B	223/233 (95%)	0.17	10 (4%) 33 16	42, 82, 147, 160	0
All	All	860/932 (92%)	0.21	52 (6%) 21 9	42, 100, 150, 195	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	14	ASN	6.8
1	A	188	MET	5.9
1	A	187	THR	5.8
1	D	175	ASN	5.0
1	A	157	PHE	4.9
1	D	68	GLY	3.8
1	C	196	GLN	3.7
2	B	24	TYR	3.6
1	D	174	VAL	3.5
1	D	35	LEU	3.5
1	D	176	PHE	3.5
1	A	12	GLN	3.4
1	D	69	VAL	3.3
1	D	66	PHE	3.3
1	D	188	MET	3.2
1	D	70	LYS	3.1
1	A	132	CYS	3.0
1	D	57	THR	3.0
2	B	171	ASN	3.0
2	B	168	LEU	3.0
1	A	214	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	140	MET	2.9
1	C	17	THR	2.8
1	D	121	GLN	2.8
1	C	21	GLU	2.7
1	A	228	GLN	2.6
2	B	174	VAL	2.5
1	A	186	GLY	2.4
1	C	185	TYR	2.4
1	D	228	GLN	2.4
2	B	203	ALA	2.4
2	B	187	THR	2.4
1	D	58	ALA	2.4
1	C	200	GLU	2.3
1	C	198	ILE	2.3
1	C	46	ASN	2.2
1	C	64	LEU	2.2
1	C	189	THR	2.2
1	D	213	TRP	2.2
2	B	175	ASN	2.2
1	D	85	PRO	2.2
1	D	165	HIS	2.2
1	D	160	LEU	2.1
1	C	55	HIS	2.1
1	D	72	THR	2.1
1	A	166	ARG	2.1
1	C	214	ALA	2.1
1	A	131	GLY	2.1
1	D	122	ILE	2.1
2	B	15	ALA	2.1
1	D	54	LEU	2.0
2	B	5	PHE	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.