



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 4IDU / pdb_00004idu
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

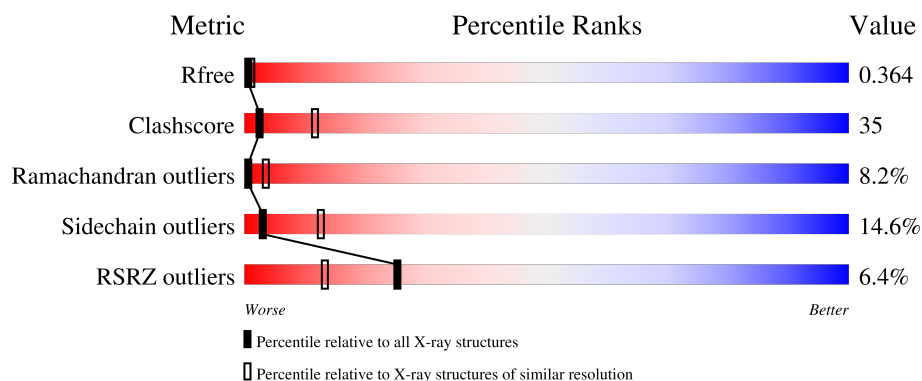
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (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 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	233	6% 34% 41% 15% • 7%
1	C	233	4% 35% 40% 11% • 12%
1	D	233	7% 47% 35% 9% • 8%
2	B	233	6% 45% 37% 13% •

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
1	A	217	Total	C	N	O	S	0	0	0
			1714	1111	288	304	11			
1	C	206	Total	C	N	O	S	0	0	0
			1635	1062	274	287	12			
1	D	214	Total	C	N	O	S	0	0	0
			1704	1111	282	299	12			

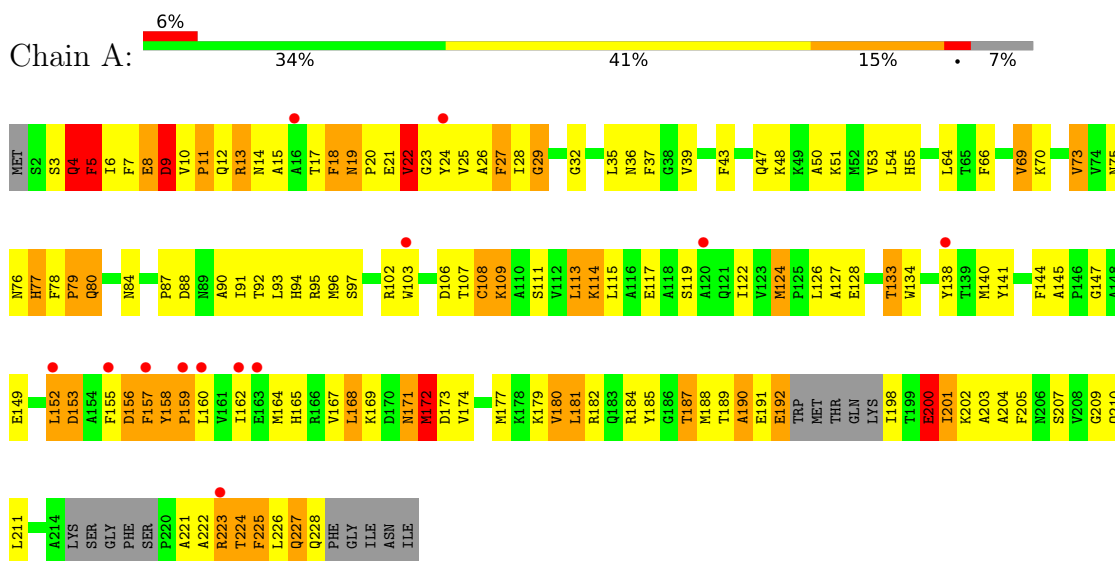
- Molecule 2 is a protein called SBV nucleoprotein.

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

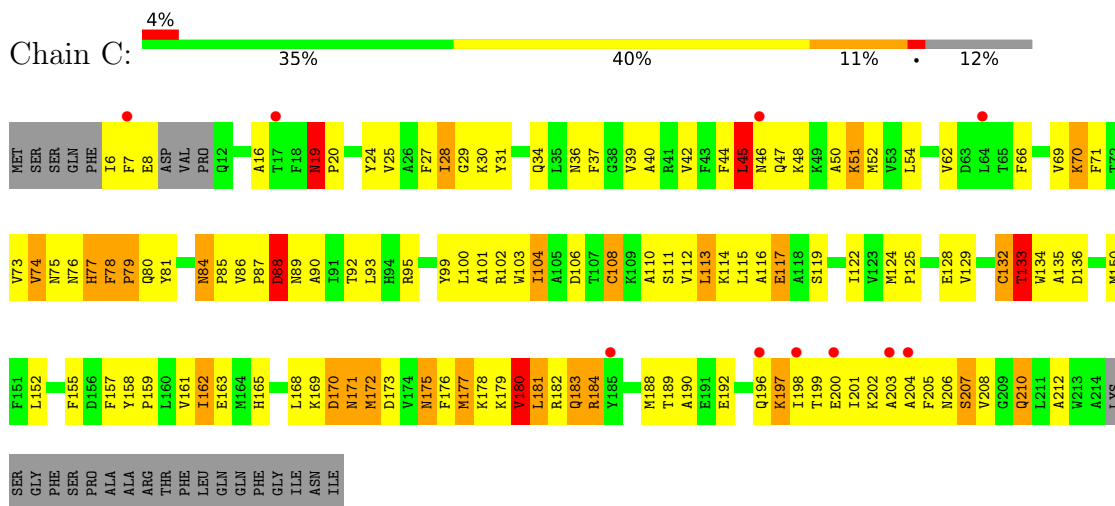
3 Residue-property plots

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: SBV nucleoprotein

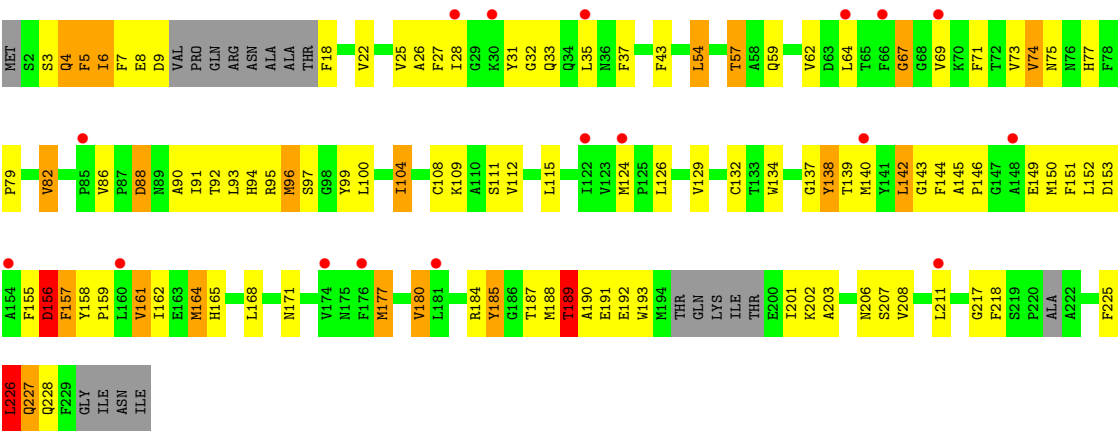


• Molecule 1: SBV nucleoprotein

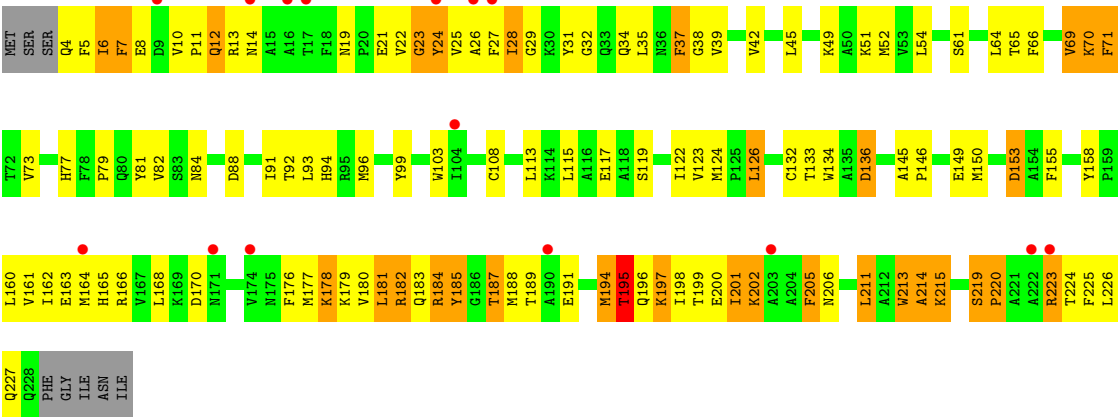


• Molecule 1: SBV nucleoprotein





● 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 29.71 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.71-3.08) 99.8 (29.71-3.08)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.06Å)	Xtriage
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	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/1756	1.01	13/2376 (0.5%)
1	C	0.67	0/1676	1.04	9/2268 (0.4%)
1	D	0.61	0/1748	0.99	3/2360 (0.1%)
2	B	0.72	0/1830	1.14	16/2475 (0.6%)
All	All	0.65	0/7010	1.05	41/9479 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	138	TYR	N-CA-C	-13.89	85.37	107.73
2	B	202	LYS	N-CA-C	11.24	125.12	111.40
2	B	28	ILE	N-CA-C	-8.41	91.84	109.34
1	C	180	VAL	N-CA-CB	8.38	125.05	111.23
1	C	50	ALA	N-CA-C	-8.32	103.99	114.56
1	C	162	ILE	N-CA-C	-8.26	102.66	110.42
2	B	195	THR	N-CA-C	8.25	128.37	110.80
2	B	12	GLN	N-CA-C	8.07	119.71	111.07
1	A	172	MET	N-CA-C	-8.00	93.75	110.80
2	B	70	LYS	N-CA-C	7.60	126.98	110.80
1	A	153	ASP	N-CA-C	7.06	120.01	111.40
1	C	170	ASP	N-CA-C	6.98	121.93	113.41
1	C	45	LEU	N-CA-C	-6.97	95.94	110.80
2	B	28	ILE	N-CA-CB	6.88	122.58	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	PHE	N-CA-C	6.74	125.16	110.80
2	B	69	VAL	N-CA-C	6.72	117.14	106.32
1	D	156	ASP	N-CA-C	6.63	124.93	110.80
1	C	46	ASN	N-CA-C	6.60	120.69	112.24
1	A	79	PRO	N-CA-C	-6.57	100.77	111.15
2	B	122	ILE	N-CA-C	6.52	117.02	107.37
1	A	79	PRO	CB-CA-C	-6.43	103.39	111.56
2	B	185	TYR	N-CA-CB	6.41	121.32	110.49
2	B	214	ALA	N-CA-C	6.38	124.40	110.80
1	A	79	PRO	CA-C-N	6.12	133.23	121.54
1	A	79	PRO	C-N-CA	6.12	133.23	121.54
2	B	178	LYS	N-CA-C	-6.06	104.99	112.38
1	A	173	ASP	N-CA-C	-6.01	100.71	110.20
2	B	205	PHE	N-CA-C	5.80	117.30	110.97
1	D	189	THR	N-CA-C	5.80	117.29	110.97
1	A	5	PHE	N-CA-C	-5.79	98.47	110.80
1	C	77	HIS	N-CA-C	-5.75	102.25	110.59
1	A	152	LEU	N-CA-C	-5.57	106.66	113.50
1	C	19	ASN	CA-C-N	-5.47	114.46	119.82
1	C	19	ASN	C-N-CA	-5.47	114.46	119.82
2	B	69	VAL	O-C-N	5.43	129.16	122.32
2	B	196	GLN	N-CA-C	-5.36	97.79	107.60
1	A	4	GLN	N-CA-C	5.28	122.05	110.80
1	A	84	ASN	N-CA-C	5.25	115.64	109.60
2	B	194	MET	N-CA-C	5.24	115.46	108.38
1	A	225	PHE	CB-CA-C	5.12	120.62	110.42
1	A	22	VAL	N-CA-C	-5.05	108.58	113.53

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 ⓘ

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	150	0
1	C	1635	0	1626	139	0
1	D	1704	0	1677	85	0
2	B	1785	0	1772	101	0
All	All	6838	0	6774	472	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 35.

All (472) 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
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:184:ARG:HB3	1:A:188:MET:HE1	1.52	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:O	1:A:29:GLY:N	2.05	0.88
1:C:196:GLN:CD	1:C:200:GLU:HG3	1.99	0.87
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: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:H	1:C:70:LYS:HD3	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
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:158:TYR:H	1:A:159:PRO:HD3	1.54	0.73
1:A:140:MET:HE1	1:A:211:LEU:HD11	1.69	0.72
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:190:ALA:HB1	1:A:191:GLU:C	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:LYS:HA	2:B:52:MET:HE3	1.74	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
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: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:77:HIS:O	1:C:78:PHE:HB3	1.96	0.66
1:D:71:PHE:CG	1:D:96:MET:HE1	2.31	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
1:C:95:ARG:HD3	1:C:150:MET:HE1	1.78	0.65
2:B:25:VAL:O	2:B:29:GLY:HA3	1.96	0.65
1:A:200:GLU:O	1:A:201:ILE:C	2.40	0.65
1:C:20:PRO:HA	1:C:24:TYR:HD1	1.60	0.65
2:B:8:GLU:HG3	2:B:179:LYS:HZ3	1.59	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
1:A:184:ARG:CB	1:A:188:MET:HE1	2.26	0.64
2:B:38:GLY:O	2:B:42:VAL:HG23	1.98	0.64
2:B:223:ARG:HD2	2:B:223:ARG:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LYS:HD3	1:C:182:ARG:HH21	1.63	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
1:C:180:VAL:C	1:C:182:ARG:H	2.08	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
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:74:VAL:HG22	1:C:92:THR:HG22	1.80	0.61
1:C:208:VAL:O	1:C:208:VAL:HG12	2.00	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: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:183:GLN:H	1:C:183:GLN:CD	2.10	0.60
1:C:48:LYS:O	1:C:52:MET:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:203:ALA:C	1:C:207:SER:HB3	2.28	0.58
1:C:54:LEU:HG	1:C:75:ASN:CG	2.29	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:D:71:PHE:CD2	1:D:96:MET:HE1	2.40	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
2:B:32:GLY:C	2:B:34:GLN:H	2.13	0.56
1:A:37:PHE:CD1	1:A:103:TRP:HZ3	2.23	0.56
2:B:91:ILE:HD11	2:B:96:MSE:HA	1.88	0.56
2:B:198:ILE:HB	2:B:201:ILE:HB	1.88	0.56
1:D:140:MET:CB	1:D:211:LEU:HD11	2.36	0.56
1:A:7:PHE:HD1	1:A:8:GLU:N	2.04	0.55
1:A:22:VAL:O	1:A:25:VAL:HG12	2.06	0.55
1:A:39:VAL:HG11	1:A:69:VAL:CG1	2.36	0.55
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:199:THR:O	1:C:202:LYS:HB3	2.07	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
1:C:88:ASP:C	1:C:90:ALA:H	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LYS:CG	1:C:198:ILE:H	2.21	0.54
1:C:177:MET:O	1:C:178:LYS:C	2.50	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
1:C:76:ASN:ND2	1:C:86:VAL:CG2	2.64	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:19:ASN:HB3	1:C:20:PRO:HD3	1.91	0.52
1:C:114:LYS:HA	1:C:117:GLU:HG2	1.90	0.52
2:B:214:ALA:O	2:B:215:LYS:C	2.52	0.52
1:A:19:ASN:C	1:A:21:GLU:H	2.17	0.52
2:B:12:GLN:C	2:B:14:ASN:H	2.15	0.52
2:B:161:VAL:HA	2:B:164:MET:HB3	1.90	0.52
1:A:22:VAL:HG13	1:A:88:ASP:O	2.09	0.52
1:A:177:MET:O	1:A:180:VAL:HG23	2.10	0.52
2:B:6:ILE:HG21	2:B:176:PHE:HZ	1.74	0.52
2:B:124:MET:CE	2:B:145:ALA:HB2	2.40	0.52
1:C:119:SER:HA	1:C:134:TRP:CE2	2.45	0.52
1:C:134:TRP:C	1:C:136:ASP:H	2.17	0.51
1:D:74:VAL:HG11	1:D:90:ALA:HB1	1.92	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
1:A:93:LEU:HA	1:A:96:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLN:NE2	1:D:62:VAL:HG13	2.25	0.51
1:D:152:LEU:HD23	1:D:159:PRO:HG2	1.92	0.51
1:C:152:LEU:HD23	1:C:157:PHE:HD1	1.75	0.51
1:D:91:ILE:HD11	1:D:96:MET:HE3	1.92	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:C:158:TYR:O	1:C:159:PRO:C	2.53	0.50
1:A:48:LYS:HZ3	1:A:126:LEU:HG	1.77	0.50
1:A:188:MET:HA	1:A:188:MET:HE3	1.93	0.50
1:D:158:TYR:O	1:D:162:ILE:HG12	2.11	0.50
1:A:226:LEU:O	1:A:227:GLN:C	2.55	0.50
1:D:67:GLY:C	1:D:69:VAL:H	2.20	0.50
2:B:150:MSE:HA	2:B:183:GLN:HG2	1.94	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: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:A:5:PHE:CD1	1:A:5:PHE:C	2.90	0.49
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
2:B:6:ILE:HG21	2:B:176:PHE:CZ	2.47	0.49
2:B:202:LYS:C	2:B:205:PHE:CD1	2.72	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
1:C:88:ASP:C	1:C:90:ALA:N	2.68	0.49
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
1:C:196:GLN:CD	1:C:200:GLU:CG	2.81	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:181:LEU:HD23	1:C:184:ARG:NH2	2.28	0.49
1:D:27:PHE:O	1:D:32:GLY:CA	2.61	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:178:LYS:CD	1:C:182:ARG:HH21	2.25	0.48
1:A:25:VAL:HG13	1:A:26:ALA:N	2.27	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
1:D:185:TYR:CD1	1:D:185:TYR:C	2.92	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
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:HG12	1:D:91:ILE:O	2.14	0.47
1:D:164:MET:SD	1:D:177:MET:HE1	2.54	0.47
1:C:113:LEU:O	1:C:116:ALA:N	2.48	0.47
1:D:27:PHE:N	1:D:27:PHE:CD1	2.81	0.47
1:D:184:ARG:HB3	1:D:187:THR:HA	1.96	0.47
1:A:224:THR:O	1:A:224:THR:OG1	2.29	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:3:SER:CB	1:D:4:GLN:HA	2.37	0.47
1:D:134:TRP:HZ3	1:D:138:TYR:HB2	1.79	0.47
2:B:22:VAL:HG12	2:B:22:VAL:O	2.14	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
2:B:178:LYS:C	2:B:182:ARG:HH21	2.22	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: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:5:PHE:CD2	1:D:6:ILE:HG13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:HIS:HA	1:D:168:LEU:HB2	1.95	0.46
1:A:128:GLU:OE1	1:A:141:TYR:OH	2.31	0.46
2:B:160:LEU:HD23	2:B:160:LEU:C	2.41	0.46
1:A:127:ALA:HB2	1:A:144:PHE:HB2	1.97	0.46
1:A:184:ARG:CG	1:A:188:MET:HE1	2.45	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:C:180:VAL:C	1:C:182:ARG:N	2.70	0.46
1:A:18:PHE:HD1	1:A:22:VAL:HG11	1.81	0.46
2:B:177:MET:C	2:B:179:LYS:N	2.70	0.46
2:B:194:MET:O	2:B:195:THR:OG1	2.29	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:162:ILE:HG12	2.16	0.46
2:B:22:VAL:CG1	2:B:88:ASP:O	2.64	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:8:GLU:CD	1:D:9:ASP:H	2.23	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:A:4:GLN:HE21	1:A:4:GLN:HA	1.82	0.45
1:A:37:PHE:CE1	1:A:103:TRP:CZ3	3.04	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
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: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
1:A:167:VAL:HA	1:A:171:ASN:C	2.42	0.45
2:B:108:CYS:HB2	2:B:115:LEU:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LYS:H	1:C:70:LYS:CD	2.23	0.44
1:D:3:SER:H	1:D:4:GLN:HB2	1.82	0.44
1:D:126:LEU:H	1:D:126:LEU:HD12	1.83	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
2:B:32:GLY:C	2:B:34:GLN:N	2.76	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:D:142:LEU:C	1:D:144:PHE:H	2.25	0.44
1:A:3:SER:OG	1:A:51:LYS:HE3	2.18	0.44
1:A:18:PHE:CD1	1:A:22:VAL:HG11	2.52	0.44
1:A:153:ASP:OD1	1:A:153:ASP:N	2.42	0.44
2:B:199:THR:O	2:B:200:GLU:HG2	2.17	0.44
1:D:161:VAL:O	1:D:164:MET:HB2	2.17	0.44
1:A:78:PHE:O	1:A:79:PRO:C	2.60	0.44
1:A:37:PHE:HB3	1:A:122:ILE:HD11	1.99	0.44
1:C:210:GLN:O	1:C:210:GLN:HG3	2.17	0.44
1:C:81:TYR:HA	1:C:84:ASN:ND2	2.33	0.43
1:A:3:SER:HB2	1:A:77:HIS:ND1	2.33	0.43
1:A:124:MET:SD	1:A:145:ALA:CB	3.04	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:110:ALA:O	1:C:111:SER:C	2.61	0.43
1:C:44:PHE:HE2	1:C:100:LEU:HB3	1.82	0.43
1:C:31:TYR:OH	1:C:71:PHE:HA	2.17	0.43
1:C:86:VAL:O	1:C:87:PRO:C	2.61	0.43
1:C:188:MET:HA	1:C:189:THR:HA	1.70	0.43
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
2:B:226:LEU:C	2:B:227:GLN:HG2	2.42	0.43
1:D:189:THR:CG2	1:D:202:LYS:HD2	2.48	0.43
1:D:225:PHE:C	1:D:227:GLN:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:5:PHE:C	1:A:5:PHE:HD1	2.26	0.42
1:D:104:ILE:HD11	1:D:142:LEU:HD11	2.01	0.42
2:B:25:VAL:HG23	2:B:26:ALA:N	2.32	0.42
2:B:27:PHE:CB	2:B:32:GLY:CA	2.89	0.42
2:B:163:GLU:OE1	2:B:166:ARG:NE	2.52	0.42
2:B:223:ARG:N	2:B:223:ARG:CD	2.74	0.42
1:A:39:VAL:HG13	1:A:66:PHE:O	2.19	0.42
2:B:223:ARG:C	2:B:225:PHE:H	2.27	0.42
1:D:95:ARG:CG	1:D:150:MET:HE1	2.49	0.42
1:C:7:PHE:CD2	1:C:8:GLU:N	2.87	0.42
2:B:8:GLU:HG3	2:B:179:LYS:HZ1	1.84	0.42
1:C:78:PHE:O	1:C:79:PRO:C	2.61	0.42
1:D:149:GLU:HG3	1:D:180:VAL:HG12	2.00	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
1:D:94:HIS:CD2	1:D:146:PRO:HB2	2.54	0.42
1:A:91:ILE:O	1:A:92:THR:C	2.63	0.42
2:B:27:PHE:O	2:B:27:PHE:CD1	2.73	0.42
2:B:223:ARG:C	2:B:225:PHE:N	2.77	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:O	1:C:208:VAL:CG1	2.67	0.42
1:D:137:GLY:HA3	1:D:140:MET:HE3	2.01	0.42
1:C:47:GLN:O	1:C:51:LYS:HB3	2.20	0.41
1:C:101:ALA:C	1:C:155:PHE:HZ	2.28	0.41
1:C:108:CYS:HB3	1:C:115:LEU:HA	2.01	0.41
1:D:109:LYS:C	1:D:111:SER:H	2.28	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:26:ALA:O	1:A:27:PHE:C	2.64	0.41
1:A:50:ALA:HA	1:A:53:VAL:HG22	2.03	0.41
1:C:27:PHE:O	1:C:29:GLY:N	2.54	0.41
1:C:180:VAL:HG23	1:C:181:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PHE:C	1:D:7:PHE:CD1	2.98	0.41
1:A:37:PHE:CD1	1:A:103:TRP:CZ3	3.07	0.41
1:A:64:LEU:HD23	1:A:66:PHE:HZ	1.85	0.41
1:A:119:SER:HA	1:A:134:TRP:CD1	2.56	0.41
2:B:37:PHE:CD1	2:B:103:TRP:CZ3	3.07	0.41
1:C:134:TRP:C	1:C:136:ASP:N	2.78	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:37:PHE:HB3	1:C:122:ILE:HD11	2.03	0.41
1:C:180:VAL:HG23	1:C:181:LEU:H	1.85	0.41
1:D:67:GLY:C	1:D:69:VAL:N	2.78	0.41
1:A:4:GLN:HE21	1:A:4:GLN:CA	2.33	0.40
1:A:140:MET:HE3	1:A:211:LEU:HD21	2.04	0.40
1:A:167:VAL:HG21	1:A:174:VAL:HG22	2.03	0.40
1:C:31:TYR:CZ	1:C:71:PHE:HA	2.56	0.40
1:C:39:VAL:HG22	1:C:66:PHE:O	2.22	0.40
1:C:172:MET:O	1:C:173:ASP:C	2.64	0.40
1:A:43:PHE:CE2	1:A:97:SER:HB3	2.57	0.40
1:A:222:ALA:HB2	2:B:181:LEU:CD2	2.51	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: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
1:A:165:HIS:NE2	1:A:169:LYS:HD2	2.36	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:21:GLU:C	2:B:23:GLY:H	2.30	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	4
1	D	206/233 (88%)	149 (72%)	47 (23%)	10 (5%)	1	9
2	B	223/233 (96%)	158 (71%)	49 (22%)	16 (7%)	1	4
All	All	842/932 (90%)	593 (70%)	180 (21%)	69 (8%)	0	3

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

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Mol	Chain	Res	Type
1	A	28	ILE
1	A	29	GLY
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 ⓘ

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%)	151 (84%)	28 (16%)	2	11
1	C	170/193 (88%)	146 (86%)	24 (14%)	3	13
1	D	178/193 (92%)	148 (83%)	30 (17%)	2	9
2	B	186/191 (97%)	164 (88%)	22 (12%)	5	20
All	All	713/770 (93%)	609 (85%)	104 (15%)	3	12

All (104) 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	22	VAL
1	A	36	ASN
1	A	69	VAL
1	A	70	LYS
1	A	73	VAL
1	A	76	ASN
1	A	77	HIS
1	A	107	THR
1	A	108	CYS
1	A	109	LYS
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

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Mol	Chain	Res	Type
1	A	187	THR
1	A	192	GLU
1	A	200	GLU
1	A	224	THR
2	B	4	GLN
2	B	10	VAL
2	B	39	VAL
2	B	45	LEU
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	181	LEU
2	B	184	ARG
2	B	189	THR
2	B	197	LYS
2	B	201	ILE
2	B	211	LEU
2	B	213	TRP
2	B	223	ARG
2	B	224	THR
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	104	ILE
1	C	106	ASP
1	C	108	CYS
1	C	113	LEU
1	C	117	GLU
1	C	128	GLU
1	C	129	VAL
1	C	133	THR

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Mol	Chain	Res	Type
1	C	168	LEU
1	C	172	MET
1	C	175	ASN
1	C	177	MET
1	C	183	GLN
1	C	197	LYS
1	C	207	SER
1	C	210	GLN
1	D	4	GLN
1	D	5	PHE
1	D	28	ILE
1	D	33	GLN
1	D	37	PHE
1	D	54	LEU
1	D	57	THR
1	D	74	VAL
1	D	77	HIS
1	D	82	VAL
1	D	86	VAL
1	D	88	ASP
1	D	96	MET
1	D	100	LEU
1	D	104	ILE
1	D	112	VAL
1	D	132	CYS
1	D	142	LEU
1	D	156	ASP
1	D	161	VAL
1	D	164	MET
1	D	171	ASN
1	D	177	MET
1	D	180	VAL
1	D	185	TYR
1	D	189	THR
1	D	201	ILE
1	D	218	PHE
1	D	226	LEU
1	D	228	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	80	GLN
1	A	175	ASN
1	A	210	GLN
2	B	12	GLN
2	B	19	ASN
2	B	46	ASN
2	B	76	ASN
2	B	77	HIS
2	B	80	GLN
2	B	94	HIS
2	B	121	GLN
2	B	196	GLN
1	C	76	ASN
1	C	84	ASN
1	C	89	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	171	ASN
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 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 ⓘ

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%)	0.61	13 (5%) 27 14	59, 102, 145, 195	0
1	C	206/233 (88%)	0.49	10 (4%) 35 18	43, 86, 119, 136	0
1	D	214/233 (91%)	0.82	17 (7%) 18 10	72, 116, 161, 175	0
2	B	223/233 (95%)	0.64	15 (6%) 24 12	42, 82, 147, 160	0
All	All	860/932 (92%)	0.64	55 (6%) 25 13	42, 100, 150, 195	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	GLN	4.7
1	A	120	ALA	4.1
1	D	160	LEU	4.0
2	B	24	TYR	3.9
1	A	157	PHE	3.6
1	D	174	VAL	3.4
1	D	140	MET	3.4
1	C	204	ALA	3.4
1	D	66	PHE	3.2
1	C	64	LEU	3.1
1	D	35	LEU	3.1
2	B	14	ASN	3.1
1	A	159	PRO	2.9
1	C	200	GLU	2.9
1	D	69	VAL	2.9
1	D	181	LEU	2.9
2	B	27	PHE	2.9
1	D	176	PHE	2.8
1	C	198	ILE	2.8
1	A	160	LEU	2.7
1	A	223	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	174	VAL	2.6
1	C	46	ASN	2.6
1	C	17	THR	2.6
2	B	26	ALA	2.5
1	C	7	PHE	2.5
1	A	16	ALA	2.4
2	B	16	ALA	2.4
1	D	148	ALA	2.4
1	D	64	LEU	2.4
2	B	104	ILE	2.4
2	B	203	ALA	2.4
2	B	190	ALA	2.4
1	A	163	GLU	2.3
1	D	122	ILE	2.3
2	B	222	ALA	2.3
2	B	9	ASP	2.3
2	B	164	MET	2.2
1	A	155	PHE	2.2
1	C	185	TYR	2.2
1	D	124	MET	2.2
1	D	211	LEU	2.2
2	B	171	ASN	2.2
1	A	138	TYR	2.2
1	D	30	LYS	2.1
1	A	103	TRP	2.1
1	D	28	ILE	2.1
2	B	223	ARG	2.1
1	D	154	ALA	2.1
1	C	203	ALA	2.1
1	D	85	PRO	2.1
1	A	152	LEU	2.0
1	A	162	ILE	2.0
1	A	24	TYR	2.0
2	B	17	THR	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 [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.