



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:16 AM UTC

PDB ID : 1KK5 / pdb_00001kk5
Title : Crystal Structure of Vat(D) (Form II)
Authors : Sugantino, M.; Roderick, S.L.
Deposited on : 2001-12-06
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

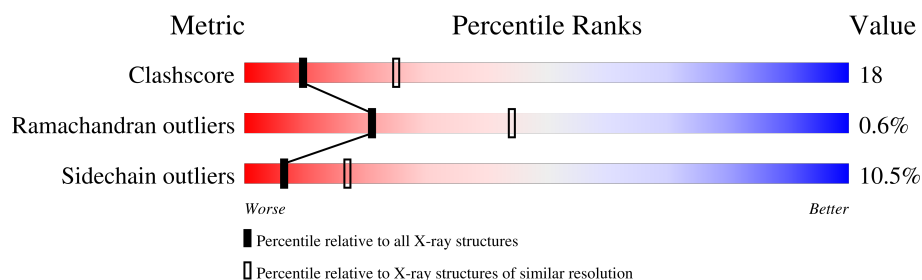
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	
1	F	209	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9850 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 STREPTOGRAMIN A ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1615	1040	266	300	9			
1	B	206	Total	C	N	O	S	0	0	0
			1615	1040	266	300	9			
1	C	206	Total	C	N	O	S	0	0	0
			1622	1044	267	302	9			
1	D	206	Total	C	N	O	S	0	0	0
			1622	1046	267	300	9			
1	E	206	Total	C	N	O	S	0	0	0
			1614	1038	265	302	9			
1	F	206	Total	C	N	O	S	0	0	0
			1612	1038	267	298	9			

- Molecule 2 is water.

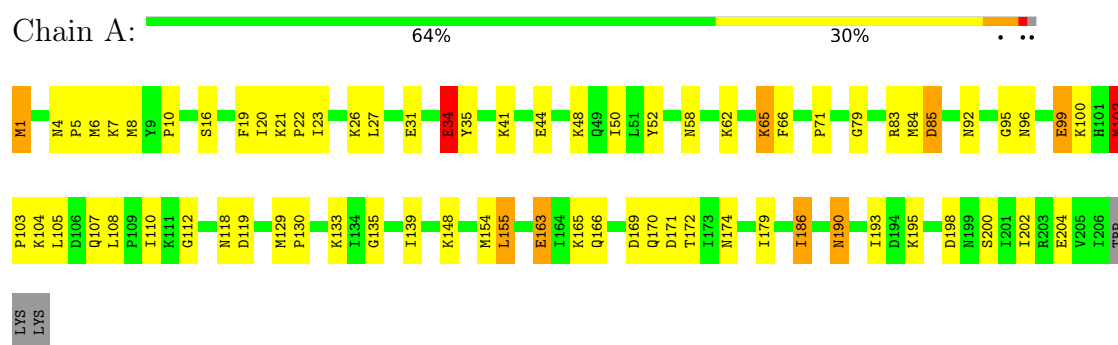
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total	O	0	0
			25	25		
2	B	29	Total	O	0	0
			29	29		
2	C	22	Total	O	0	0
			22	22		
2	D	23	Total	O	0	0
			23	23		
2	E	26	Total	O	0	0
			26	26		
2	F	25	Total	O	0	0
			25	25		

3 Residue-property plots [i](#)

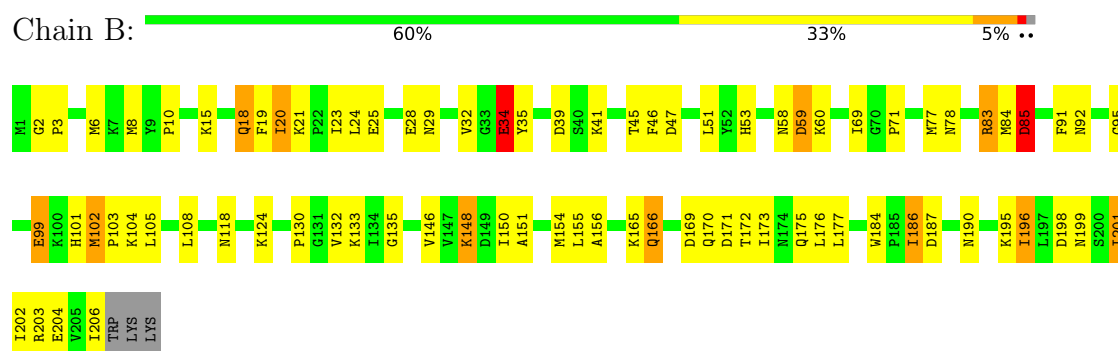
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

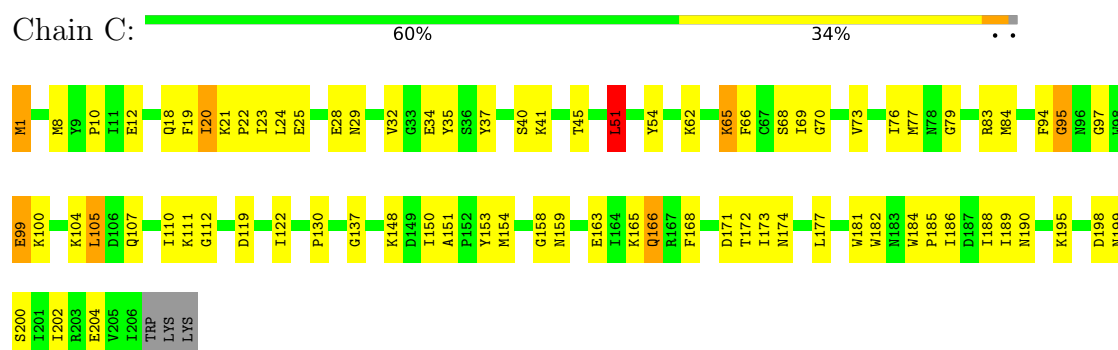
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



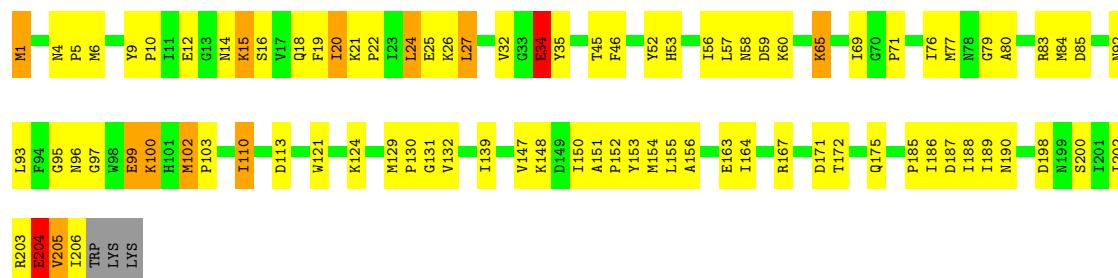
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



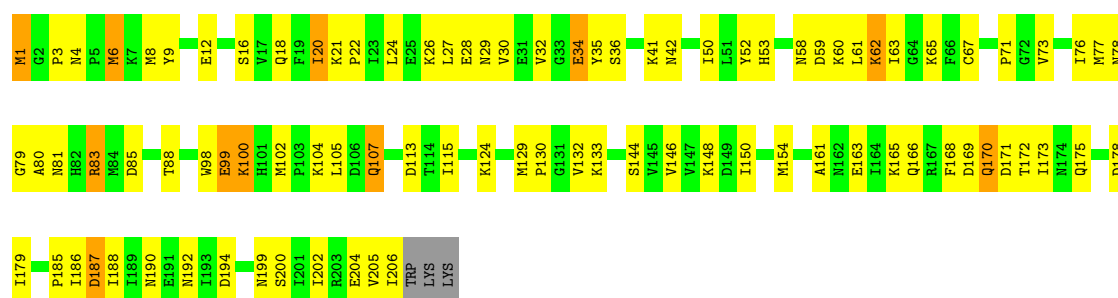
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



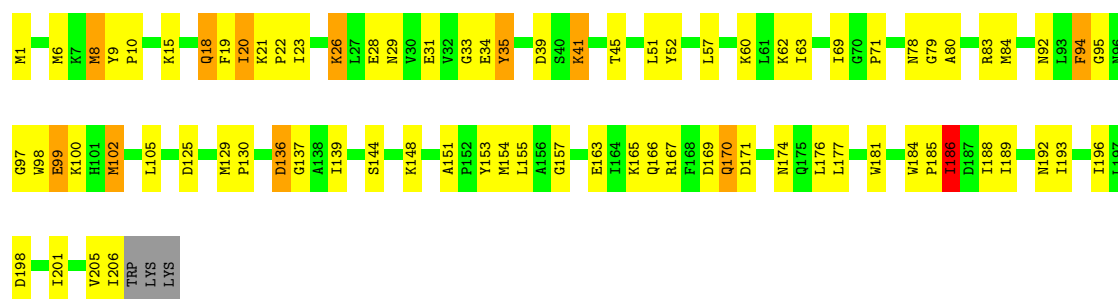
● Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain D:  57% 35% 5% ..

● Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain E:  55% 38% 5% .

● Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain F:  60% 33% 5% .

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	185.80Å 185.80Å 186.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.9 (99.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9850	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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	0.57	1/1654 (0.1%)	1.01	5/2246 (0.2%)
1	B	0.58	0/1654	1.04	14/2246 (0.6%)
1	C	0.64	3/1661 (0.2%)	1.01	6/2254 (0.3%)
1	D	0.62	1/1660 (0.1%)	1.09	15/2252 (0.7%)
1	E	0.57	0/1653	1.03	6/2246 (0.3%)
1	F	0.56	0/1651	1.02	8/2241 (0.4%)
All	All	0.59	5/9933 (0.1%)	1.03	54/13485 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	ASN	C-N	9.03	1.51	1.34
1	D	203	ARG	CA-C	7.15	1.62	1.52
1	C	77	MET	SD-CE	-5.67	1.65	1.79
1	C	158	GLY	C-N	-5.35	1.28	1.33
1	A	102	MET	SD-CE	5.05	1.92	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	GLU	N-CA-C	9.78	121.89	111.03
1	B	34	GLU	N-CA-C	9.26	120.98	111.07
1	D	20	ILE	N-CA-C	9.04	119.85	110.36
1	E	34	GLU	N-CA-C	8.98	120.84	111.14
1	D	34	GLU	N-CA-C	8.81	120.57	110.97
1	D	205	VAL	N-CA-C	-8.43	105.11	113.20
1	F	35	TYR	N-CA-C	7.73	122.35	113.15
1	E	83	ARG	N-CA-C	-7.72	99.85	110.35
1	D	85	ASP	N-CA-C	-7.10	104.50	113.02
1	D	203	ARG	NE-CZ-NH1	-7.02	114.48	121.50
1	D	58	ASN	N-CA-C	6.90	121.01	111.90
1	A	135	GLY	N-CA-C	6.84	119.85	112.33
1	F	20	ILE	N-CA-C	6.79	116.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASN	N-CA-C	6.40	120.43	112.24
1	D	203	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	B	20	ILE	N-CA-C	6.17	116.92	110.62
1	E	20	ILE	N-CA-C	6.16	118.79	111.09
1	C	20	ILE	N-CA-C	6.11	116.29	110.42
1	D	46	PHE	N-CA-C	6.04	119.74	112.38
1	F	51	LEU	N-CA-C	6.03	119.88	110.17
1	A	20	ILE	N-CA-C	6.03	119.52	111.44
1	D	24	LEU	N-CA-C	5.98	117.60	111.14
1	F	78	ASN	N-CA-C	5.95	119.64	112.38
1	D	204	GLU	N-CA-C	5.90	120.00	113.21
1	C	35	TYR	N-CA-C	5.67	119.18	112.72
1	F	60	LYS	N-CA-C	5.65	118.90	110.14
1	D	84	MET	N-CA-C	5.52	119.11	111.71
1	E	107	GLN	N-CA-C	-5.52	106.68	113.41
1	C	51	LEU	N-CA-C	5.51	118.72	109.95
1	D	83	ARG	N-CA-C	-5.51	102.73	110.50
1	C	185	PRO	N-CA-C	-5.50	102.56	111.14
1	C	84	MET	N-CA-C	5.50	119.78	112.30
1	B	104	LYS	N-CA-C	-5.42	103.23	110.55
1	B	146	VAL	N-CA-C	5.40	116.13	107.98
1	D	59	ASP	N-CA-C	-5.38	101.69	110.20
1	B	78	ASN	N-CA-C	5.33	119.66	113.20
1	B	51	LEU	N-CA-C	5.29	118.34	110.14
1	B	46	PHE	N-CA-C	5.28	118.51	111.75
1	B	85	ASP	N-CA-C	-5.28	106.80	113.18
1	F	83	ARG	N-CA-C	-5.27	102.06	109.96
1	B	130	PRO	N-CA-C	5.24	119.53	111.21
1	F	94	PHE	N-CA-C	5.23	119.64	113.16
1	E	35	TYR	N-CA-C	5.19	119.70	113.17
1	D	187	ASP	N-CA-C	-5.18	105.71	111.36
1	D	10	PRO	N-CA-CB	5.18	108.69	103.25
1	A	186	ILE	N-CA-C	5.17	117.51	111.05
1	C	83	ARG	N-CA-C	-5.16	102.75	110.23
1	E	73	VAL	N-CA-C	-5.16	102.94	109.80
1	B	83	ARG	N-CA-C	-5.11	103.41	110.35
1	F	84	MET	N-CA-C	5.08	118.58	111.56
1	B	92	ASN	N-CA-C	5.05	117.44	111.33
1	B	135	GLY	N-CA-C	5.05	119.02	112.25
1	B	2	GLY	CA-C-N	5.02	125.23	120.31
1	B	2	GLY	C-N-CA	5.02	125.23	120.31

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	1615	0	1592	55	0
1	B	1615	0	1592	52	0
1	C	1622	0	1602	52	0
1	D	1622	0	1610	71	0
1	E	1614	0	1580	61	0
1	F	1612	0	1590	56	0
2	A	25	0	0	3	0
2	B	29	0	0	4	0
2	C	22	0	0	1	0
2	D	23	0	0	1	0
2	E	26	0	0	8	0
2	F	25	0	0	1	0
All	All	9850	0	9566	341	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (341) 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:F:154:MET:HE3	1:F:163:GLU:HB3	1.53	0.90
1:D:95:GLY:HA2	1:D:99:GLU:HG3	1.51	0.89
1:F:95:GLY:HA2	1:F:99:GLU:HG3	1.54	0.87
1:C:151:ALA:HB3	1:C:154:MET:HG3	1.60	0.84
1:D:154:MET:HE2	1:D:163:GLU:HG2	1.59	0.82
1:A:1:MET:HE3	1:A:190:ASN:OD1	1.79	0.82
1:D:185:PRO:HD2	1:D:188:ILE:HD12	1.60	0.81
1:A:154:MET:HE3	1:A:163:GLU:HG2	1.63	0.79
1:B:95:GLY:HA2	1:B:99:GLU:HG3	1.63	0.79
1:E:172:THR:HG23	1:E:202:ILE:HD13	1.66	0.78
1:F:41:LYS:HB2	1:F:71:PRO:HB2	1.65	0.78
1:B:23:ILE:HG22	1:B:24:LEU:HD23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HG22	1:C:24:LEU:HD23	1.69	0.75
1:C:95:GLY:HA2	1:C:99:GLU:HG3	1.68	0.75
1:B:196:ILE:HG13	1:B:201:ILE:HD12	1.69	0.74
1:F:184:TRP:CZ3	1:F:201:ILE:HD11	2.22	0.74
1:A:6:MET:HA	1:A:6:MET:HE2	1.69	0.74
1:A:139:ILE:HB	1:A:155:LEU:HD13	1.69	0.73
1:E:102:MET:HE3	2:E:2139:HOH:O	1.87	0.73
1:D:97:GLY:N	1:D:99:GLU:OE2	2.22	0.71
1:E:21:LYS:HB2	2:E:2075:HOH:O	1.92	0.70
1:B:171:ASP:O	1:B:175:GLN:HG3	1.93	0.69
1:D:19:PHE:O	1:D:22:PRO:HD2	1.93	0.69
1:C:34:GLU:HG2	1:C:65:LYS:HD2	1.74	0.68
1:E:83:ARG:HG2	2:E:2025:HOH:O	1.92	0.68
1:F:139:ILE:HB	1:F:155:LEU:HD12	1.76	0.68
1:C:195:LYS:HG2	1:C:200:SER:OG	1.94	0.68
1:D:71:PRO:O	1:D:124:LYS:HB2	1.94	0.67
1:D:172:THR:HG23	1:D:202:ILE:CD1	2.24	0.67
1:F:20:ILE:HD11	1:F:69:ILE:HD12	1.78	0.66
1:D:204:GLU:OE1	1:D:204:GLU:HA	1.95	0.66
1:B:35:TYR:OH	1:B:186:ILE:HD13	1.96	0.66
1:F:8:MET:HE3	1:F:9:TYR:CE1	2.30	0.66
1:A:83:ARG:HG2	2:A:2011:HOH:O	1.94	0.66
1:B:184:TRP:CH2	1:B:201:ILE:HD11	2.31	0.66
1:E:178:ASP:CG	2:E:2080:HOH:O	2.38	0.66
1:F:92:ASN:HA	1:F:98:TRP:O	1.96	0.65
1:D:57:LEU:HD22	1:D:110:ILE:HD11	1.78	0.65
1:B:172:THR:HG23	1:B:202:ILE:HD11	1.78	0.64
1:D:25:GLU:C	1:D:27:LEU:H	2.03	0.64
1:E:52:TYR:CD1	1:E:80:ALA:HB2	2.31	0.64
1:A:169:ASP:OD1	1:A:171:ASP:HB3	1.97	0.64
1:F:8:MET:HG2	1:F:23:ILE:HG12	1.80	0.63
1:B:28:GLU:O	1:B:29:ASN:HB2	1.98	0.63
1:C:20:ILE:HD11	1:C:69:ILE:HD12	1.80	0.63
1:F:151:ALA:HB3	1:F:154:MET:HG3	1.81	0.63
1:A:1:MET:CE	1:A:190:ASN:OD1	2.47	0.63
1:F:20:ILE:CD1	1:F:69:ILE:HD12	2.29	0.63
1:A:34:GLU:HG2	1:A:65:LYS:HD2	1.80	0.62
1:F:92:ASN:HB2	1:F:102:MET:HE3	1.80	0.62
1:F:181:TRP:CE3	1:F:196:ILE:HD13	2.34	0.62
1:E:8:MET:HE2	1:E:9:TYR:CE1	2.34	0.62
1:F:92:ASN:HD22	1:F:102:MET:CE	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:THR:HG23	1:D:202:ILE:HD13	1.81	0.62
1:A:41:LYS:HB2	1:A:71:PRO:HB2	1.81	0.61
1:A:26:LYS:O	1:A:27:LEU:HD23	1.99	0.61
1:A:133:LYS:NZ	2:A:2086:HOH:O	2.32	0.61
1:A:195:LYS:NZ	1:A:204:GLU:HG3	2.14	0.61
1:B:184:TRP:CZ3	1:B:201:ILE:HD11	2.35	0.61
1:C:195:LYS:HD3	1:C:204:GLU:OE1	2.01	0.61
1:E:21:LYS:HB3	1:E:22:PRO:HD3	1.82	0.61
1:E:24:LEU:HD12	1:E:32:VAL:HG21	1.82	0.61
1:A:92:ASN:HD22	1:A:102:MET:HE2	1.65	0.61
1:D:186:ILE:HD11	1:E:98:TRP:CZ2	2.36	0.60
1:E:20:ILE:HG22	1:E:32:VAL:HG11	1.82	0.60
1:D:95:GLY:HA2	1:D:99:GLU:CG	2.26	0.60
1:F:205:VAL:O	1:F:206:ILE:C	2.44	0.60
1:C:51:LEU:HD12	1:C:76:ILE:HD13	1.82	0.60
1:D:154:MET:HE2	1:D:163:GLU:CG	2.30	0.60
1:B:60:LYS:HE3	2:B:2087:HOH:O	2.01	0.60
1:C:69:ILE:HG12	1:C:122:ILE:HD12	1.83	0.59
1:D:151:ALA:HB3	1:D:154:MET:HG3	1.84	0.59
1:D:204:GLU:OE1	1:D:204:GLU:CA	2.50	0.59
1:D:139:ILE:HD12	1:D:167:ARG:HD2	1.84	0.59
1:D:1:MET:HE3	1:D:190:ASN:CG	2.28	0.59
1:D:52:TYR:CD1	1:D:80:ALA:HB2	2.38	0.59
1:D:92:ASN:OD1	1:D:102:MET:HE2	2.03	0.59
1:E:175:GLN:O	1:E:179:ILE:HG13	2.03	0.58
1:C:104:LYS:HB2	1:C:107:GLN:OE1	2.04	0.58
1:F:31:GLU:OE2	1:F:62:LYS:HE2	2.03	0.58
1:A:154:MET:CE	1:A:163:GLU:HG2	2.32	0.58
1:C:154:MET:HE2	1:C:163:GLU:HB3	1.86	0.58
1:D:186:ILE:HD11	1:E:98:TRP:HZ2	1.69	0.57
1:F:170:GLN:O	1:F:174:ASN:ND2	2.37	0.57
1:E:161:ALA:HB3	2:E:2076:HOH:O	2.03	0.57
1:F:144:SER:OG	1:F:157:GLY:HA2	2.04	0.57
1:F:196:ILE:HG12	1:F:201:ILE:HD12	1.86	0.57
1:C:51:LEU:HD12	1:C:76:ILE:CD1	2.34	0.57
1:E:132:VAL:HG11	1:E:146:VAL:HG12	1.87	0.57
1:D:93:LEU:HG	1:D:93:LEU:O	2.03	0.57
1:B:6:MET:HE1	1:B:21:LYS:HE2	1.87	0.57
1:E:199:ASN:O	1:E:202:ILE:HD12	2.05	0.57
1:F:184:TRP:CH2	1:F:201:ILE:HD11	2.39	0.57
1:C:34:GLU:HG2	1:C:65:LYS:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:PRO:HG2	1:E:124:LYS:HB2	1.88	0.56
1:E:187:ASP:CG	2:E:2160:HOH:O	2.47	0.56
1:F:92:ASN:HD22	1:F:102:MET:HE2	1.69	0.56
1:C:24:LEU:HD12	1:C:32:VAL:HG21	1.86	0.56
1:B:186:ILE:HG13	1:B:190:ASN:ND2	2.21	0.56
1:B:85:ASP:OD1	1:B:85:ASP:N	2.34	0.56
1:E:1:MET:HG2	1:F:97:GLY:HA3	1.86	0.56
1:B:195:LYS:NZ	1:B:204:GLU:HG3	2.21	0.56
1:B:18:GLN:OE1	1:B:45:THR:HA	2.06	0.56
1:A:83:ARG:NE	1:A:85:ASP:OD2	2.36	0.55
1:B:39:ASP:O	1:B:71:PRO:HB3	2.06	0.55
1:C:19:PHE:O	1:C:22:PRO:HD2	2.06	0.55
1:E:100:LYS:C	1:E:102:MET:H	2.13	0.55
1:A:198:ASP:HB3	2:A:2041:HOH:O	2.06	0.55
1:B:172:THR:HG23	1:B:202:ILE:CD1	2.37	0.55
1:A:165:LYS:HG2	1:A:166:GLN:O	2.06	0.55
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.88	0.55
1:A:41:LYS:HG3	1:A:41:LYS:O	2.07	0.55
1:D:198:ASP:C	1:D:198:ASP:OD1	2.49	0.55
1:D:121:TRP:HE3	1:D:139:ILE:HG12	1.71	0.55
1:C:37:TYR:CE2	1:C:68:SER:HA	2.42	0.54
1:C:10:PRO:HB3	1:C:19:PHE:CE1	2.42	0.54
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.89	0.54
1:D:6:MET:N	1:D:6:MET:HE2	2.22	0.54
1:B:91:PHE:HB2	2:B:2044:HOH:O	2.06	0.54
1:C:165:LYS:HG2	1:C:166:GLN:N	2.22	0.54
1:D:139:ILE:HB	1:D:155:LEU:HD13	1.89	0.54
1:F:136:ASP:O	1:F:153:TYR:N	2.38	0.54
1:E:154:MET:HE3	1:E:163:GLU:HB3	1.90	0.54
1:C:171:ASP:O	1:C:174:ASN:HB2	2.08	0.53
1:D:139:ILE:HB	1:D:155:LEU:CD1	2.38	0.53
1:D:186:ILE:HD13	2:D:2117:HOH:O	2.07	0.53
1:E:36:SER:HB3	1:E:67:CYS:HB2	1.90	0.53
1:F:15:LYS:HE3	2:F:2178:HOH:O	2.09	0.53
1:E:21:LYS:HB3	1:E:22:PRO:CD	2.39	0.53
1:B:59:ASP:OD1	1:B:59:ASP:N	2.39	0.53
1:E:26:LYS:O	1:E:27:LEU:HD23	2.09	0.53
1:E:20:ILE:CG2	1:E:32:VAL:HG11	2.38	0.52
1:D:53:HIS:CD2	1:D:77:MET:HG3	2.44	0.52
1:F:185:PRO:O	1:F:186:ILE:C	2.53	0.52
1:D:24:LEU:O	1:D:27:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASN:ND2	2:B:2087:HOH:O	2.42	0.52
1:C:198:ASP:OD1	1:C:198:ASP:C	2.52	0.52
1:A:66:PHE:O	1:A:119:ASP:HA	2.09	0.52
1:F:18:GLN:OE1	1:F:45:THR:HA	2.10	0.52
1:C:1:MET:N	2:C:2065:HOH:O	2.42	0.52
1:B:53:HIS:CG	1:B:77:MET:HG3	2.45	0.52
1:C:97:GLY:N	1:C:99:GLU:OE2	2.37	0.52
1:D:1:MET:HE3	1:D:190:ASN:OD1	2.11	0.51
1:E:185:PRO:HD2	1:E:188:ILE:HD12	1.92	0.51
1:D:35:TYR:CZ	1:D:186:ILE:HD12	2.46	0.51
1:D:113:ASP:O	1:D:131:GLY:HA2	2.10	0.51
1:A:95:GLY:HA2	1:A:99:GLU:HG2	1.92	0.51
1:D:24:LEU:O	1:D:25:GLU:C	2.53	0.51
1:F:35:TYR:OH	1:F:186:ILE:HD12	2.09	0.51
1:B:186:ILE:CG1	1:B:190:ASN:HD21	2.22	0.51
1:B:196:ILE:CG1	1:B:201:ILE:HD12	2.38	0.51
1:B:186:ILE:CG1	1:B:190:ASN:ND2	2.74	0.50
1:B:186:ILE:HG12	1:B:190:ASN:HD21	1.75	0.50
1:D:9:TYR:CE2	1:D:15:LYS:HA	2.46	0.50
1:A:104:LYS:HB2	1:A:107:GLN:HG3	1.92	0.50
1:A:195:LYS:HZ1	1:A:204:GLU:HG3	1.76	0.50
1:C:104:LYS:HB2	1:C:107:GLN:HG3	1.92	0.50
1:D:172:THR:HG23	1:D:202:ILE:HD11	1.92	0.50
1:A:52:TYR:HB3	1:A:79:GLY:HA3	1.93	0.50
1:D:20:ILE:HG22	1:D:32:VAL:HG11	1.94	0.50
1:D:205:VAL:O	1:D:205:VAL:HG12	2.11	0.50
1:D:205:VAL:O	1:D:206:ILE:HB	2.10	0.50
1:A:21:LYS:N	1:A:22:PRO:HD2	2.26	0.50
1:E:29:ASN:O	1:E:60:LYS:HA	2.11	0.50
1:F:171:ASP:C	1:F:171:ASP:OD1	2.55	0.50
1:A:165:LYS:HG2	1:A:166:GLN:N	2.25	0.50
1:B:151:ALA:HB3	1:B:154:MET:HG3	1.94	0.50
1:C:104:LYS:CB	1:C:107:GLN:HG3	2.42	0.50
1:D:34:GLU:HG2	1:D:65:LYS:CD	2.42	0.50
1:A:110:ILE:HG22	1:A:112:GLY:H	1.77	0.49
1:A:186:ILE:O	1:A:190:ASN:HB2	2.12	0.49
1:C:95:GLY:HA2	1:C:99:GLU:CG	2.39	0.49
1:D:4:ASN:OD1	1:D:6:MET:HB2	2.12	0.49
1:D:25:GLU:O	1:D:27:LEU:N	2.44	0.49
1:A:95:GLY:HA2	1:A:99:GLU:CG	2.43	0.49
1:A:104:LYS:O	1:A:105:LEU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLY:O	1:D:96:ASN:HB2	2.12	0.49
1:E:3:PRO:HG3	1:F:94:PHE:HB3	1.94	0.49
1:E:188:ILE:O	1:E:192:ASN:ND2	2.46	0.49
1:D:34:GLU:HG2	1:D:65:LYS:HD3	1.94	0.49
1:F:23:ILE:O	1:F:26:LYS:HE3	2.11	0.49
1:C:28:GLU:O	1:C:29:ASN:HB2	2.12	0.49
1:A:6:MET:HE1	1:A:21:LYS:HD3	1.93	0.49
1:E:30:VAL:HG23	1:E:53:HIS:HE1	1.78	0.49
1:F:137:GLY:HA3	1:F:153:TYR:CE2	2.48	0.49
1:E:53:HIS:CD2	1:E:77:MET:HG3	2.46	0.49
1:A:52:TYR:HB3	1:A:79:GLY:CA	2.42	0.49
1:A:139:ILE:HB	1:A:155:LEU:CD1	2.42	0.49
1:C:188:ILE:O	1:C:189:ILE:C	2.56	0.49
1:D:25:GLU:C	1:D:27:LEU:N	2.69	0.49
1:F:92:ASN:ND2	1:F:102:MET:HE2	2.27	0.49
1:D:205:VAL:O	1:D:206:ILE:CB	2.60	0.49
1:F:6:MET:HE1	1:F:21:LYS:HE2	1.94	0.49
1:C:18:GLN:OE1	1:C:45:THR:HA	2.14	0.48
1:D:24:LEU:O	1:D:27:LEU:N	2.46	0.48
1:A:103:PRO:HB2	1:A:108:LEU:HD21	1.95	0.48
1:D:52:TYR:HB3	1:D:79:GLY:HA3	1.95	0.48
1:B:83:ARG:HG2	1:B:85:ASP:OD1	2.14	0.48
1:D:154:MET:HE2	1:D:163:GLU:HB3	1.95	0.48
1:F:185:PRO:HD2	1:F:188:ILE:HD12	1.96	0.48
1:C:111:LYS:HD2	1:C:130:PRO:HB2	1.96	0.48
1:C:186:ILE:O	1:C:190:ASN:HB2	2.13	0.48
1:E:4:ASN:OD1	1:E:6:MET:HB2	2.14	0.48
1:A:172:THR:HG23	1:A:202:ILE:HD13	1.95	0.47
1:C:20:ILE:CD1	1:C:69:ILE:HD12	2.42	0.47
1:C:173:ILE:HG22	1:C:177:LEU:HD12	1.96	0.47
1:C:94:PHE:O	1:C:95:GLY:C	2.57	0.47
1:A:202:ILE:O	1:A:202:ILE:HG22	2.14	0.47
1:C:66:PHE:O	1:C:119:ASP:HA	2.14	0.47
1:B:53:HIS:CD2	1:B:77:MET:HG3	2.49	0.47
1:A:200:SER:C	1:A:202:ILE:H	2.22	0.47
1:B:187:ASP:HA	1:B:190:ASN:HD22	1.80	0.47
1:B:195:LYS:HZ2	1:B:204:GLU:HG3	1.79	0.47
1:B:186:ILE:HG23	1:B:187:ASP:N	2.29	0.47
1:E:60:LYS:O	1:E:113:ASP:HB3	2.14	0.47
1:A:44:GLU:N	1:A:44:GLU:OE1	2.48	0.47
1:D:5:PRO:C	1:D:6:MET:HE2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:OE2	1:A:62:LYS:HE2	2.15	0.47
1:C:200:SER:C	1:C:202:ILE:N	2.72	0.47
1:E:169:ASP:O	1:E:171:ASP:N	2.48	0.46
1:D:150:ILE:HD13	1:D:156:ALA:CB	2.45	0.46
1:F:139:ILE:HD12	1:F:167:ARG:HD2	1.96	0.46
1:A:200:SER:C	1:A:202:ILE:N	2.71	0.46
1:C:172:THR:HG23	1:C:202:ILE:HD13	1.96	0.46
1:F:154:MET:HE3	1:F:163:GLU:CB	2.34	0.46
1:B:10:PRO:HG3	1:B:19:PHE:CE1	2.51	0.46
1:C:65:LYS:HE2	1:C:182:TRP:O	2.15	0.46
1:A:104:LYS:O	1:A:107:GLN:N	2.36	0.46
1:B:132:VAL:HG12	1:B:133:LYS:N	2.30	0.46
1:E:52:TYR:HB3	1:E:79:GLY:HA3	1.97	0.46
1:D:18:GLN:OE1	1:D:45:THR:HA	2.16	0.45
1:B:169:ASP:OD1	1:B:171:ASP:HB2	2.16	0.45
1:D:200:SER:C	1:D:202:ILE:N	2.73	0.45
1:A:103:PRO:CG	1:A:108:LEU:HD21	2.46	0.45
1:E:78:ASN:HB3	1:E:81:ASN:ND2	2.31	0.45
1:F:57:LEU:HD11	1:F:79:GLY:HA2	1.98	0.45
1:A:172:THR:HG23	1:A:202:ILE:CD1	2.46	0.45
1:C:137:GLY:HA3	1:C:153:TYR:CE2	2.51	0.45
1:E:62:LYS:HD2	1:E:115:ILE:HG12	1.97	0.45
1:E:115:ILE:HD12	1:E:133:LYS:HE2	1.97	0.45
1:E:53:HIS:CG	1:E:77:MET:HG3	2.52	0.45
1:E:76:ILE:O	1:E:130:PRO:HG3	2.16	0.45
1:E:169:ASP:C	1:E:171:ASP:N	2.73	0.45
1:A:129:MET:HB3	1:A:130:PRO:HD2	1.98	0.45
1:B:170:GLN:O	1:B:171:ASP:C	2.59	0.45
1:F:57:LEU:CD1	1:F:79:GLY:HA2	2.47	0.45
1:E:99:GLU:H	1:E:99:GLU:HG3	1.42	0.45
1:E:172:THR:HG23	1:E:202:ILE:CD1	2.40	0.45
1:C:54:TYR:CE1	1:C:79:GLY:HA3	2.51	0.45
1:D:188:ILE:O	1:D:189:ILE:C	2.58	0.45
1:D:204:GLU:CD	1:D:204:GLU:N	2.74	0.45
1:E:169:ASP:C	1:E:171:ASP:H	2.25	0.44
1:B:176:LEU:HD23	1:B:176:LEU:HA	1.82	0.44
1:B:150:ILE:HD13	1:B:156:ALA:CB	2.47	0.44
1:B:198:ASP:O	1:B:199:ASN:HB2	2.17	0.44
1:F:198:ASP:OD1	1:F:198:ASP:C	2.60	0.44
1:B:20:ILE:CD1	1:B:69:ILE:HD12	2.47	0.44
1:E:204:GLU:C	1:E:206:ILE:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CZ	1:A:186:ILE:HD12	2.53	0.44
1:A:193:ILE:HG21	1:B:101:HIS:CD2	2.53	0.44
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.81	0.44
1:E:41:LYS:HG2	1:E:42:ASN:ND2	2.32	0.44
1:F:39:ASP:O	1:F:71:PRO:HB3	2.17	0.44
1:E:129:MET:O	1:E:132:VAL:HG23	2.18	0.44
1:B:154:MET:SD	1:B:166:GLN:HG3	2.58	0.43
1:A:195:LYS:HZ2	1:A:204:GLU:HG3	1.82	0.43
1:C:104:LYS:O	1:C:105:LEU:C	2.60	0.43
1:C:200:SER:O	1:C:202:ILE:N	2.51	0.43
1:B:148:LYS:NZ	2:B:2171:HOH:O	2.51	0.43
1:D:20:ILE:HG23	1:D:24:LEU:HG	2.00	0.43
1:D:52:TYR:HD1	1:D:76:ILE:HG23	1.82	0.43
1:D:129:MET:HG3	1:D:147:VAL:HG12	2.01	0.43
1:B:20:ILE:HG22	1:B:32:VAL:HG11	1.99	0.43
1:D:152:PRO:O	1:D:153:TYR:C	2.61	0.43
1:F:137:GLY:HA3	1:F:153:TYR:CD2	2.54	0.43
1:F:139:ILE:HB	1:F:155:LEU:CD1	2.47	0.43
1:A:96:ASN:N	1:A:96:ASN:HD22	2.17	0.43
1:D:14:ASN:OD1	1:D:14:ASN:C	2.62	0.43
1:F:52:TYR:CD1	1:F:80:ALA:HB2	2.54	0.43
1:A:10:PRO:HB3	1:A:19:PHE:CE1	2.54	0.43
1:D:9:TYR:CD2	1:D:15:LYS:HA	2.54	0.43
1:D:21:LYS:HB3	1:D:22:PRO:HD3	1.99	0.43
1:F:129:MET:HB3	1:F:130:PRO:HD2	2.01	0.43
1:D:20:ILE:CD1	1:D:69:ILE:HD12	2.49	0.42
1:D:97:GLY:O	1:D:100:LYS:HG3	2.18	0.42
1:D:171:ASP:O	1:D:175:GLN:HG3	2.19	0.42
1:E:204:GLU:O	1:E:206:ILE:N	2.52	0.42
1:B:173:ILE:HG22	1:B:177:LEU:HD12	2.00	0.42
1:C:154:MET:HE2	1:C:163:GLU:HG2	2.00	0.42
1:F:33:GLY:N	1:F:63:ILE:O	2.51	0.42
1:A:99:GLU:H	1:A:99:GLU:HG3	1.38	0.42
1:E:8:MET:HE2	1:E:8:MET:HB3	1.71	0.42
1:A:4:ASN:O	1:A:6:MET:N	2.52	0.42
1:A:8:MET:HE3	1:A:23:ILE:HG12	2.00	0.42
1:A:65:LYS:H	1:A:65:LYS:HG2	1.71	0.42
1:A:31:GLU:HB2	1:A:62:LYS:HG2	2.01	0.42
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.92	0.42
1:E:100:LYS:C	1:E:102:MET:N	2.77	0.42
1:D:139:ILE:HD12	1:D:167:ARG:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:HB2	1:B:71:PRO:HB2	2.02	0.42
1:B:45:THR:OG1	1:B:47:ASP:OD1	2.32	0.42
1:C:110:ILE:HG22	1:C:112:GLY:H	1.85	0.42
1:E:30:VAL:HG23	1:E:53:HIS:CE1	2.54	0.42
1:B:202:ILE:O	1:B:206:ILE:CB	2.67	0.42
1:F:153:TYR:CZ	1:F:176:LEU:HD13	2.54	0.42
1:C:154:MET:HE2	1:C:163:GLU:CG	2.50	0.42
1:D:92:ASN:HB2	1:D:102:MET:HE2	2.01	0.42
1:E:32:VAL:HG13	1:E:63:ILE:HB	2.01	0.42
1:E:36:SER:CB	1:E:67:CYS:HB2	2.50	0.41
1:F:192:ASN:O	1:F:193:ILE:C	2.61	0.41
1:B:34:GLU:HB2	1:B:35:TYR:CD1	2.56	0.41
1:F:10:PRO:HB3	1:F:19:PHE:CE1	2.56	0.41
1:C:200:SER:C	1:C:202:ILE:H	2.28	0.41
1:A:174:ASN:HD22	1:A:174:ASN:HA	1.73	0.41
1:B:3:PRO:HG3	1:C:94:PHE:HB3	2.02	0.41
1:C:168:PHE:CZ	1:C:199:ASN:ND2	2.88	0.41
1:E:168:PHE:O	1:E:173:ILE:HD11	2.20	0.41
1:C:104:LYS:HB2	1:C:107:GLN:CG	2.51	0.41
1:E:104:LYS:O	1:E:105:LEU:C	2.62	0.41
1:E:200:SER:C	1:E:202:ILE:N	2.78	0.41
1:C:181:TRP:HA	1:C:184:TRP:CE2	2.56	0.41
1:E:52:TYR:HB3	1:E:79:GLY:CA	2.51	0.41
1:F:151:ALA:O	1:F:154:MET:HB2	2.20	0.41
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.80	0.41
1:F:184:TRP:HB2	1:F:189:ILE:HG13	2.03	0.41
1:F:28:GLU:O	1:F:29:ASN:HB2	2.19	0.41
1:F:41:LYS:NZ	1:F:125:ASP:OD1	2.45	0.41
1:D:129:MET:HB3	1:D:130:PRO:CD	2.51	0.40
1:D:152:PRO:O	1:D:154:MET:HG2	2.20	0.40
1:F:169:ASP:OD1	1:F:171:ASP:HB3	2.21	0.40
1:E:59:ASP:OD1	1:E:59:ASP:N	2.55	0.40
1:A:198:ASP:OD1	1:A:198:ASP:C	2.64	0.40
1:E:58:ASN:HA	2:E:2073:HOH:O	2.21	0.40
1:E:104:LYS:O	1:E:107:GLN:N	2.37	0.40
1:E:190:ASN:ND2	2:E:2138:HOH:O	2.54	0.40
1:F:18:GLN:HE21	1:F:18:GLN:HB3	1.74	0.40
1:F:21:LYS:HB3	1:F:22:PRO:HD3	2.03	0.40
1:C:70:GLY:O	1:C:73:VAL:HG23	2.22	0.40
1:C:172:THR:O	1:C:173:ILE:C	2.64	0.40
1:D:102:MET:HG3	1:D:103:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:HE2	1:D:163:GLU:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/209 (98%)	182 (89%)	21 (10%)	1 (0%)	24	48
1	B	204/209 (98%)	194 (95%)	10 (5%)	0	100	100
1	C	204/209 (98%)	191 (94%)	12 (6%)	1 (0%)	24	48
1	D	204/209 (98%)	184 (90%)	19 (9%)	1 (0%)	24	48
1	E	204/209 (98%)	194 (95%)	8 (4%)	2 (1%)	12	32
1	F	204/209 (98%)	189 (93%)	13 (6%)	2 (1%)	12	32
All	All	1224/1254 (98%)	1134 (93%)	83 (7%)	7 (1%)	21	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	VAL
1	D	26	LYS
1	E	170	GLN
1	F	34	GLU
1	F	186	ILE
1	C	95	GLY
1	A	5	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	174/183 (95%)	155 (89%)	19 (11%)	6	16
1	B	174/183 (95%)	154 (88%)	20 (12%)	5	14
1	C	175/183 (96%)	160 (91%)	15 (9%)	10	25
1	D	175/183 (96%)	158 (90%)	17 (10%)	8	20
1	E	173/183 (94%)	149 (86%)	24 (14%)	3	9
1	F	173/183 (94%)	158 (91%)	15 (9%)	9	24
All	All	1044/1098 (95%)	934 (90%)	110 (10%)	6	17

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LYS
1	A	16	SER
1	A	34	GLU
1	A	48	LYS
1	A	50	ILE
1	A	65	LYS
1	A	84	MET
1	A	85	ASP
1	A	99	GLU
1	A	100	LYS
1	A	102	MET
1	A	118	ASN
1	A	148	LYS
1	A	155	LEU
1	A	163	GLU
1	A	170	GLN
1	A	179	ILE
1	A	190	ASN
1	B	8	MET
1	B	15	LYS
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	25	GLU
1	B	34	GLU
1	B	59	ASP
1	B	84	MET
1	B	85	ASP
1	B	99	GLU
1	B	102	MET
1	B	118	ASN
1	B	124	LYS
1	B	148	LYS
1	B	155	LEU
1	B	165	LYS
1	B	166	GLN
1	B	186	ILE
1	B	196	ILE
1	B	201	ILE
1	B	203	ARG
1	C	1	MET
1	C	8	MET
1	C	12	GLU
1	C	25	GLU
1	C	40	SER
1	C	41	LYS
1	C	51	LEU
1	C	62	LYS
1	C	65	LYS
1	C	99	GLU
1	C	100	LYS
1	C	105	LEU
1	C	148	LYS
1	C	150	ILE
1	C	166	GLN
1	D	1	MET
1	D	12	GLU
1	D	15	LYS
1	D	16	SER
1	D	27	LEU
1	D	34	GLU
1	D	56	ILE
1	D	60	LYS
1	D	65	LYS
1	D	99	GLU

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Mol	Chain	Res	Type
1	D	100	LYS
1	D	102	MET
1	D	110	ILE
1	D	132	VAL
1	D	148	LYS
1	D	164	ILE
1	D	204	GLU
1	E	1	MET
1	E	6	MET
1	E	12	GLU
1	E	16	SER
1	E	18	GLN
1	E	28	GLU
1	E	34	GLU
1	E	50	ILE
1	E	61	LEU
1	E	62	LYS
1	E	65	LYS
1	E	85	ASP
1	E	88	THR
1	E	99	GLU
1	E	100	LYS
1	E	144	SER
1	E	148	LYS
1	E	150	ILE
1	E	165	LYS
1	E	166	GLN
1	E	170	GLN
1	E	186	ILE
1	E	187	ASP
1	E	194	ASP
1	F	1	MET
1	F	8	MET
1	F	18	GLN
1	F	26	LYS
1	F	41	LYS
1	F	99	GLU
1	F	100	LYS
1	F	102	MET
1	F	105	LEU
1	F	136	ASP
1	F	148	LYS

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Mol	Chain	Res	Type
1	F	165	LYS
1	F	166	GLN
1	F	170	GLN
1	F	186	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	96	ASN
1	A	101	HIS
1	A	166	GLN
1	A	170	GLN
1	A	174	ASN
1	A	192	ASN
1	B	49	GLN
1	B	58	ASN
1	B	96	ASN
1	B	101	HIS
1	B	143	ASN
1	B	166	GLN
1	B	170	GLN
1	B	174	ASN
1	B	190	ASN
1	B	192	ASN
1	C	143	ASN
1	C	166	GLN
1	C	170	GLN
1	C	174	ASN
1	D	166	GLN
1	D	174	ASN
1	E	42	ASN
1	E	81	ASN
1	E	92	ASN
1	E	166	GLN
1	E	170	GLN
1	E	174	ASN
1	E	192	ASN
1	F	92	ASN
1	F	170	GLN
1	F	174	ASN
1	F	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.