



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:04 PM UTC

PDB ID : 1KTK / pdb_00001ktk
Title : Complex of Streptococcal pyrogenic enterotoxin C (SpeC) with a human T cell receptor beta chain (Vbeta2.1)
Authors : Sundberg, E.J.; Li, H.; Llera, A.S.; McCormick, J.K.; Tormo, J.; Karjalainen, K.; Schlievert, P.M.; Mariuzza, R.A.
Deposited on : 2002-01-16
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

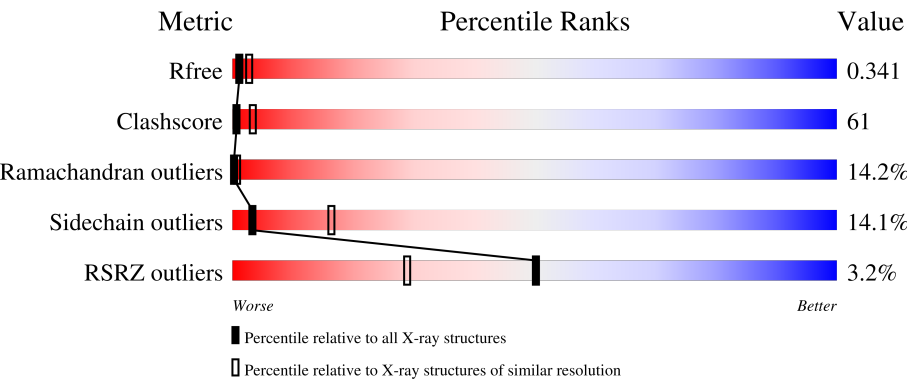
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	208	28% 50% 15% . .
1	B	208	3% 20% 60% 15% . .
1	C	208	29% 54% 14% .
1	D	208	33% 46% 14% . 5%
2	E	247	4% 18% 45% 28% 9%

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Mol	Chain	Length	Quality of chain
2	F	247	6% 14% 22% 20% • 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9511 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 Exotoxin type C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1664	1062	275	323	4			
1	B	200	Total	C	N	O	S	0	0	0
			1624	1042	267	311	4			
1	C	208	Total	C	N	O	S	0	0	0
			1699	1083	279	333	4			
1	D	198	Total	C	N	O	S	0	0	0
			1601	1028	267	303	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASP	ASN	conflict	UNP P13380
B	26	ASP	ASN	conflict	UNP P13380
C	26	ASP	ASN	conflict	UNP P13380
D	26	ASP	ASN	conflict	UNP P13380

- Molecule 2 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	247	Total	C	N	O	S	0	0	0
			1879	1178	324	370	7			
2	F	144	Total	C	N	O	S	0	0	0
			1044	656	180	203	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	ARG	TRP	conflict	UNP P01850
E	13	ALA	CYS	conflict	UNP P01850
E	50	ALA	ASN	conflict	UNP P01850
E	95	LEU	-	insertion	UNP P01850

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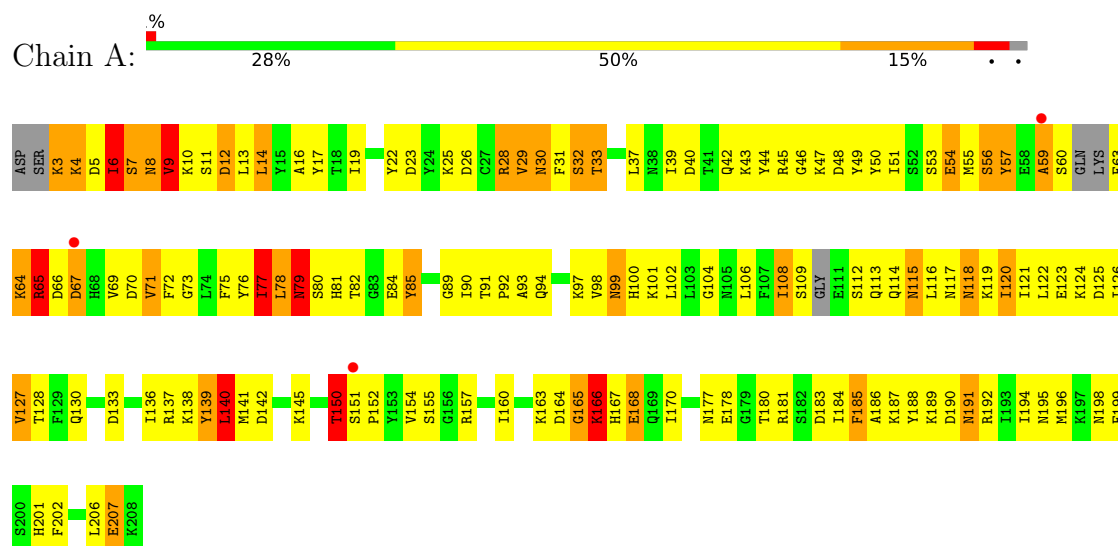
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Chain	Residue	Modelled	Actual	Comment	Reference
E	96	ALA	ARG	conflict	UNP P01850
E	99	GLY	GLU	conflict	UNP P01850
E	99	GLY	THR	conflict	UNP P01850
E	101	SER	-	insertion	UNP P01850
E	102	THR	-	insertion	UNP P01850
E	?	-	PRO	deletion	UNP P01850
E	?	-	LYS	deletion	UNP P01850
E	?	-	ASN	deletion	UNP P01850
E	105	THR	GLU	conflict	UNP P01850
E	107	TYR	PHE	conflict	UNP P01850
E	?	-	VAL	deletion	UNP P01850
E	191	ALA	CYS	conflict	UNP P01850
F	10	ARG	TRP	conflict	UNP P01850
F	13	ALA	CYS	conflict	UNP P01850
F	50	ALA	ASN	conflict	UNP P01850
F	96	LEU	-	insertion	UNP P01850
F	97	ALA	ARG	conflict	UNP P01850
F	98	GLY	GLU	conflict	UNP P01850
F	100	GLY	THR	conflict	UNP P01850
F	102	SER	-	insertion	UNP P01850
F	103	THR	-	insertion	UNP P01850
F	?	-	PRO	deletion	UNP P01850
F	?	-	LYS	deletion	UNP P01850
F	?	-	ASN	deletion	UNP P01850
F	105	THR	GLU	conflict	UNP P01850
F	107	TYR	PHE	conflict	UNP P01850
F	?	-	VAL	deletion	UNP P01850
F	191	ALA	CYS	conflict	UNP P01850

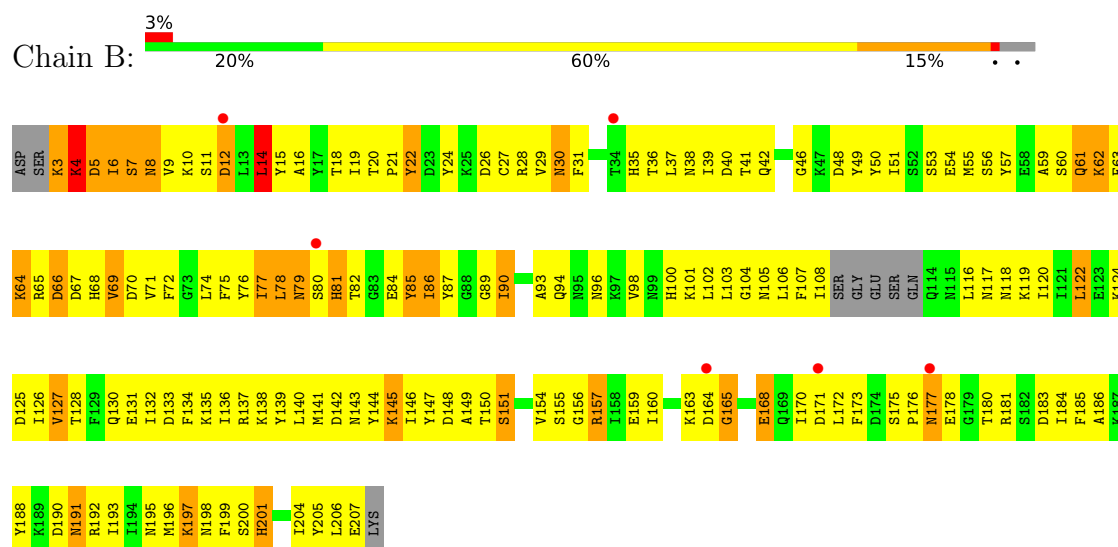
3 Residue-property plots

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: Exotoxin type C

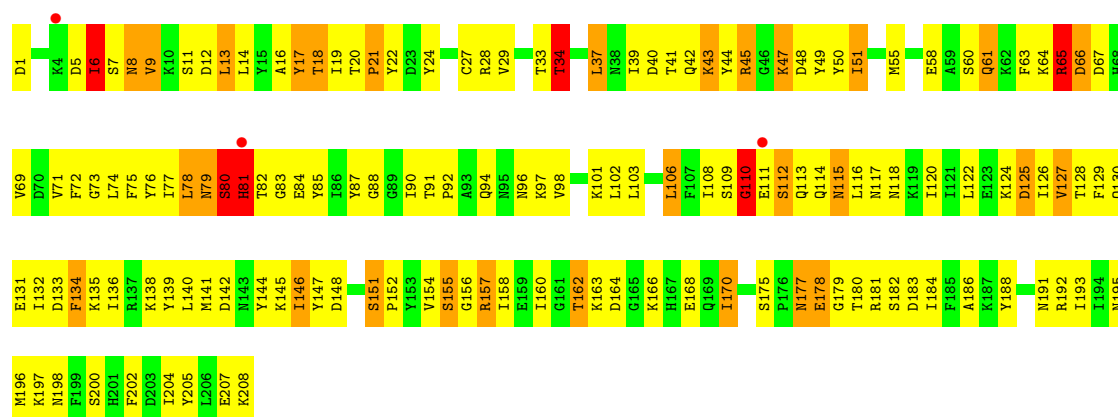


• Molecule 1: Exotoxin type C

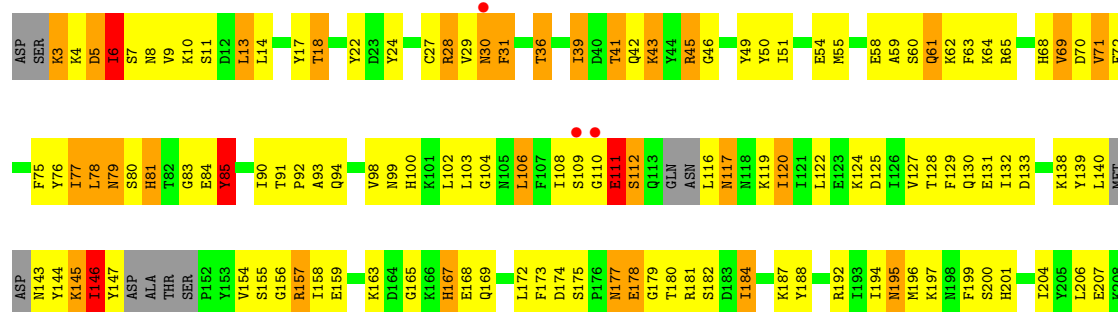


• Molecule 1: Exotoxin type C

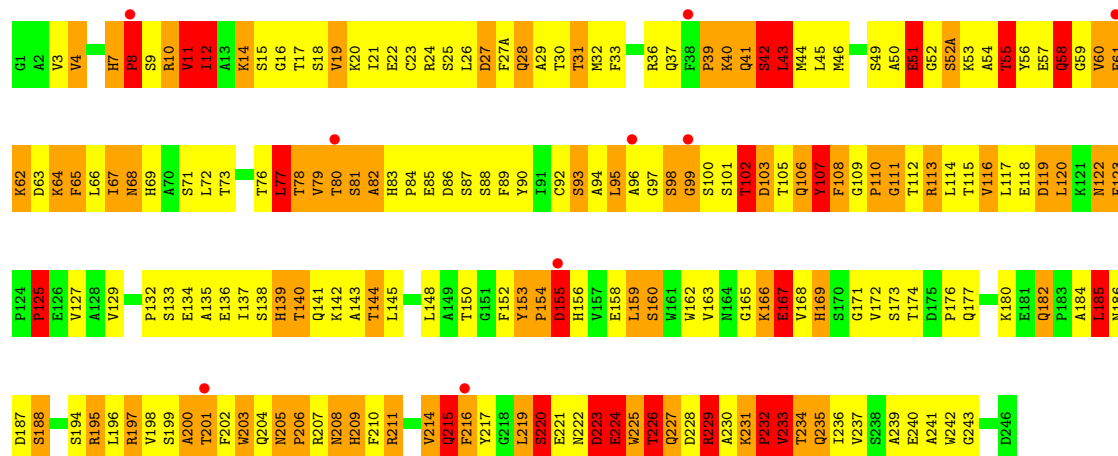
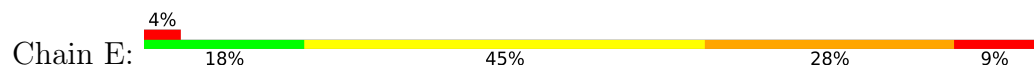




- Molecule 1: Exotoxin type C

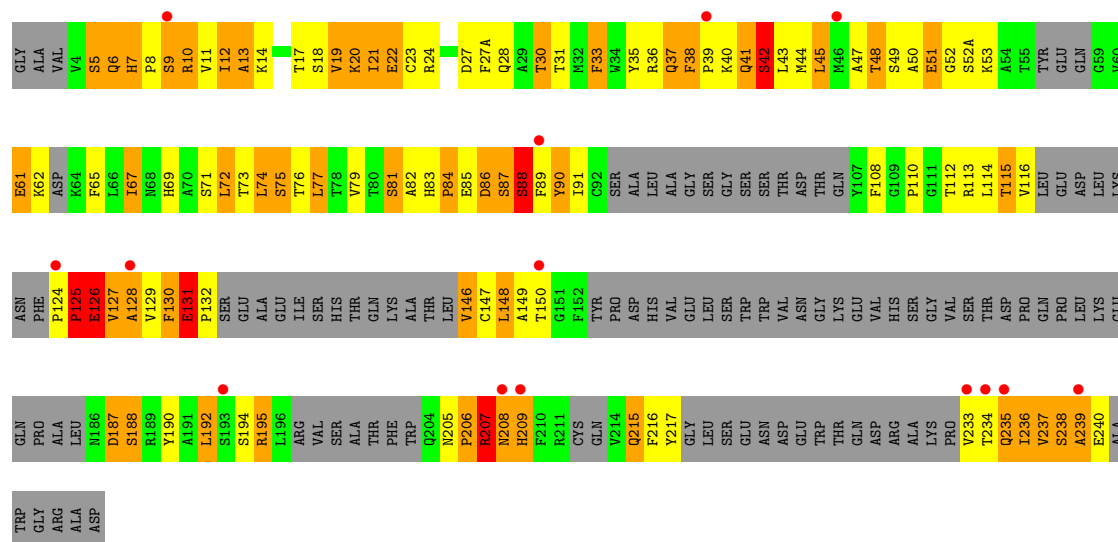


- Molecule 2: T-cell receptor beta chain



- Molecule 2: T-cell receptor beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.38Å 146.76Å 135.69Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 6.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (6.00-3.00) 85.4 (6.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.326 , 0.334 0.334 , 0.341	Depositor DCC
R_{free} test set	1941 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9511	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.76	0/1697	1.28	17/2282 (0.7%)
1	B	0.59	0/1659	1.15	12/2240 (0.5%)
1	C	0.76	0/1735	1.23	23/2338 (1.0%)
1	D	0.60	0/1633	1.21	16/2197 (0.7%)
2	E	0.67	0/1924	1.52	38/2620 (1.5%)
2	F	0.55	0/1055	1.42	26/1421 (1.8%)
All	All	0.67	0/9703	1.31	132/13098 (1.0%)

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	F	0	1

There are no bond length outliers.

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	HIS	CA-C-N	20.49	145.46	119.84
2	E	7	HIS	C-N-CA	20.49	145.46	119.84
1	D	80	SER	N-CA-C	-18.06	88.37	112.03
2	F	85	GLU	N-CA-C	-12.80	85.23	108.02
2	E	225	TRP	N-CA-C	12.22	127.78	111.28
1	B	4	LYS	N-CA-C	10.91	134.03	110.80
2	E	203	TRP	N-CA-C	-10.61	99.86	113.12
2	E	215	GLN	N-CA-C	10.15	125.98	113.50
2	F	38	PHE	CA-C-N	-10.02	110.61	120.83
2	F	38	PHE	C-N-CA	-10.02	110.61	120.83
1	C	9	VAL	N-CA-C	-9.66	103.25	111.56
1	A	79	ASN	N-CA-C	9.62	131.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	N-CA-C	-9.42	96.12	109.69
2	E	65	PHE	N-CA-C	-9.36	90.86	110.80
2	E	7	HIS	C-N-CD	-9.25	87.06	125.00
2	E	214	VAL	N-CA-C	-8.84	95.27	108.97
2	F	12	ILE	N-CA-C	8.62	115.43	106.21
1	D	111	GLU	N-CA-C	-8.61	92.46	110.80
1	A	57	TYR	N-CA-C	8.46	120.68	110.19
2	E	109	GLY	CA-C-N	8.43	130.38	119.84
2	E	109	GLY	C-N-CA	8.43	130.38	119.84
2	E	220	SER	N-CA-C	8.42	128.73	110.80
2	E	200	ALA	N-CA-C	-8.31	101.91	110.97
2	F	82	ALA	N-CA-C	-8.22	98.12	109.95
2	E	201	THR	N-CA-C	-8.11	99.06	110.50
2	E	166	LYS	N-CA-C	8.10	122.65	109.85
1	C	79	ASN	N-CA-C	8.08	128.01	110.80
2	E	134	GLU	N-CA-C	-7.83	103.94	113.97
2	F	88	SER	N-CA-C	-7.71	94.37	110.80
2	F	72	LEU	N-CA-C	-7.69	103.00	112.38
2	F	215	GLN	N-CA-C	7.60	120.42	108.79
1	A	78	LEU	N-CA-C	7.57	118.52	108.07
2	E	8	PRO	N-CA-C	-7.52	96.98	112.47
2	F	190	TYR	N-CA-C	7.47	118.13	108.34
1	D	178	GLU	N-CA-C	-7.46	103.19	113.56
1	C	198	ASN	N-CA-C	-7.44	104.23	113.38
1	A	59	ALA	N-CA-C	-7.40	102.83	112.68
2	F	90	TYR	N-CA-C	-7.34	98.08	109.76
2	F	132	PRO	N-CA-CB	7.22	110.94	103.00
1	B	85	TYR	N-CA-C	7.18	120.94	109.24
2	F	22	GLU	N-CA-C	7.10	120.55	107.99
1	D	109	SER	N-CA-C	7.09	119.35	109.15
1	C	151	SER	CA-C-N	7.01	128.23	120.45
1	C	151	SER	C-N-CA	7.01	128.23	120.45
1	A	141	MET	N-CA-C	-6.99	103.27	111.03
2	F	6	GLN	N-CA-C	-6.98	99.98	109.54
1	D	195	ASN	N-CA-C	-6.97	99.18	110.20
2	E	106	GLN	N-CA-C	6.92	119.65	107.61
1	D	62	LYS	N-CA-C	6.89	119.42	109.71
1	A	139	TYR	N-CA-C	-6.82	97.43	108.41
1	B	12	ASP	N-CA-C	-6.80	105.11	113.41
1	C	43	LYS	N-CA-C	-6.72	104.56	112.89
1	C	151	SER	N-CA-C	6.67	120.22	110.14
1	B	127	VAL	N-CA-C	6.64	117.60	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	SER	N-CA-C	-6.63	96.69	110.80
2	E	107	TYR	N-CA-C	6.62	124.91	110.80
1	C	78	LEU	N-CA-C	6.57	120.23	109.85
1	A	71	VAL	N-CA-C	6.55	117.28	108.11
1	B	5	ASP	N-CA-C	6.54	124.72	110.80
2	E	219	LEU	N-CA-C	6.52	119.06	108.76
2	F	86	ASP	N-CA-C	6.51	121.10	112.25
1	C	42	GLN	N-CA-C	6.50	120.81	113.01
2	E	102	THR	N-CA-C	6.50	124.64	110.80
2	E	209	HIS	N-CA-C	6.49	119.65	110.50
2	E	43	LEU	N-CA-C	6.48	124.60	110.80
1	B	79	ASN	N-CA-C	6.45	124.53	110.80
1	C	114	GLN	N-CA-C	-6.44	99.62	109.41
2	E	42	SER	N-CA-C	6.37	124.38	110.80
1	C	34	THR	N-CA-C	-6.37	104.77	113.30
2	F	84	PRO	N-CA-C	6.36	125.57	112.47
2	E	7	HIS	N-CA-C	6.35	123.84	109.81
1	D	79	ASN	N-CA-C	6.35	124.32	110.80
1	B	62	LYS	N-CA-C	-6.33	105.20	114.39
1	A	120	ILE	N-CA-C	-6.32	98.36	107.78
1	C	115	ASN	N-CA-C	6.26	119.74	109.85
2	F	216	PHE	N-CA-C	-6.12	99.09	108.76
1	D	17	TYR	N-CA-C	6.11	120.35	113.02
2	E	185	LEU	N-CA-C	-6.11	97.79	110.80
1	C	51	ILE	N-CA-C	-6.10	99.70	108.48
2	F	209	HIS	N-CA-C	6.08	118.42	109.24
2	F	45	LEU	N-CA-C	6.07	117.41	108.86
2	F	207	ARG	N-CA-C	6.01	123.60	110.80
2	E	105	THR	N-CA-C	5.99	118.95	110.50
2	F	74	LEU	N-CA-C	5.98	117.77	110.41
2	E	226	THR	N-CA-C	5.96	123.50	110.80
1	A	118	ASN	N-CA-C	5.92	123.40	110.80
2	E	58	GLN	N-CA-C	5.91	123.39	110.80
2	E	11	VAL	N-CA-C	5.89	121.60	109.34
2	E	24	ARG	N-CA-C	5.87	118.24	108.20
1	D	18	THR	N-CA-C	-5.85	97.65	108.24
1	B	22	TYR	N-CA-C	-5.84	100.97	110.20
1	C	81	HIS	N-CA-C	-5.83	98.39	110.80
1	D	69	VAL	N-CA-C	5.83	117.75	108.89
2	F	38	PHE	N-CA-C	-5.79	97.01	109.81
2	E	119	ASP	N-CA-C	-5.74	103.73	111.54
1	A	42	GLN	N-CA-C	5.70	118.27	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LEU	N-CA-C	-5.69	98.69	110.80
2	F	19	VAL	N-CA-C	5.68	117.18	108.71
1	D	71	VAL	N-CA-C	5.67	116.76	108.53
1	D	36	THR	N-CA-C	5.62	116.78	108.86
1	A	166	LYS	N-CA-C	5.60	117.91	107.99
1	C	125	ASP	N-CA-C	-5.57	106.32	113.23
1	D	28	ARG	N-CA-C	5.55	118.27	109.50
1	D	30	ASN	N-CA-CB	-5.55	102.37	110.53
1	C	162	THR	N-CA-C	-5.54	101.14	109.95
1	C	110	GLY	N-CA-C	-5.50	100.14	113.18
1	A	165	GLY	N-CA-C	5.49	126.20	113.18
1	B	173	PHE	N-CA-C	5.49	117.57	110.65
2	E	223	ASP	N-CA-C	5.46	122.43	110.80
1	B	143	ASN	N-CA-C	5.45	120.05	112.90
2	E	171	GLY	N-CA-C	-5.42	108.14	115.36
2	E	12	ILE	N-CA-C	5.42	120.61	109.34
2	E	224	GLU	N-CA-C	-5.40	99.29	110.80
1	C	17	TYR	N-CA-C	5.37	119.94	112.90
1	A	56	SER	N-CA-C	-5.36	103.27	110.24
2	F	42	SER	N-CA-C	5.35	122.20	110.80
1	A	6	ILE	N-CA-C	5.31	120.39	109.34
2	F	12	ILE	CB-CA-C	-5.27	107.32	113.22
1	D	85	TYR	N-CA-C	5.27	117.55	109.07
1	A	45	ARG	N-CA-C	5.25	119.74	113.23
2	F	128	ALA	N-CA-C	-5.25	101.78	109.81
2	F	13	ALA	CA-C-O	-5.23	115.30	121.16
2	E	182	GLN	CA-C-N	5.23	125.52	119.93
2	E	182	GLN	C-N-CA	5.23	125.52	119.93
1	C	8	ASN	N-CA-C	-5.19	105.84	113.72
1	B	3	LYS	CA-C-N	5.17	131.40	121.54
1	B	3	LYS	C-N-CA	5.17	131.40	121.54
1	C	21	PRO	N-CA-C	5.14	119.38	111.57
1	D	39	ILE	N-CA-C	5.13	116.75	108.85
1	C	66	ASP	N-CA-C	5.08	118.61	111.90
1	C	37	LEU	N-CA-C	-5.06	100.92	109.07
2	E	77	LEU	N-CA-C	-5.04	100.69	108.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	130	PHE	Sidechain

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	1664	0	1608	193	0
1	B	1624	0	1554	224	0
1	C	1699	0	1634	150	0
1	D	1601	0	1539	165	0
2	E	1879	0	1775	306	1
2	F	1044	0	965	150	0
All	All	9511	0	9075	1142	1

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 61.

All (1142) 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:E:57:GLU:OE2	2:E:63:ASP:HB2	1.43	1.17
1:A:180:THR:HG22	2:E:54:ALA:HB2	1.30	1.10
2:E:15:SER:HA	2:E:82:ALA:O	1.52	1.09
2:E:79:VAL:HG13	2:E:80:THR:H	1.17	1.08
2:F:86:ASP:HB3	2:F:115:THR:HA	1.15	1.08
2:F:36:ARG:HG2	2:F:37:GLN:H	1.14	1.07
2:E:12:ILE:H	2:E:12:ILE:HD12	1.15	1.05
1:C:63:PHE:O	1:C:64:LYS:HG3	1.55	1.04
2:E:43:LEU:HD11	2:E:108:PHE:HZ	1.16	1.04
2:E:62:LYS:HA	2:E:62:LYS:HE2	1.40	1.01
1:D:69:VAL:HG21	1:D:90:ILE:HG23	1.38	1.01
1:B:124:LYS:HB2	1:B:127:VAL:HG22	1.40	1.01
2:F:19:VAL:HB	2:F:79:VAL:HG22	1.44	1.00
1:A:69:VAL:HG21	1:A:90:ILE:HG23	1.39	0.99
1:D:102:LEU:HD12	1:D:120:ILE:HG22	1.43	0.99
2:F:129:VAL:O	2:F:130:PHE:HA	1.64	0.97
1:B:51:ILE:HD13	1:B:84:GLU:HB2	1.45	0.97
1:B:8:ASN:O	1:B:12:ASP:HB2	1.64	0.96
1:C:69:VAL:HG21	1:C:90:ILE:HG23	1.45	0.96
2:F:30:THR:HG23	2:F:31:THR:H	1.31	0.96
1:A:28:ARG:HG2	1:A:40:ASP:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TYR:HA	1:B:181:ARG:HB3	1.46	0.96
1:A:94:GLN:HE22	1:A:125:ASP:H	1.14	0.95
1:B:78:LEU:N	2:F:52:GLY:HA3	1.80	0.95
1:C:141:MET:HE3	1:C:147:TYR:HD2	1.28	0.94
2:E:219:LEU:HD22	2:E:220:SER:H	1.30	0.94
1:B:108:ILE:HG12	1:B:206:LEU:HB2	1.49	0.94
2:E:18:SER:HA	2:E:80:THR:O	1.67	0.94
2:E:43:LEU:HD11	2:E:108:PHE:CZ	2.02	0.94
1:C:156:GLY:HA2	1:C:157:ARG:NH2	1.82	0.93
1:D:102:LEU:HD11	1:D:122:LEU:HG	1.50	0.93
1:C:6:ILE:HG23	1:C:7:SER:H	1.31	0.93
1:B:14:LEU:HD23	1:B:15:TYR:N	1.83	0.92
2:E:158:GLU:HB3	2:E:215:GLN:HB3	1.51	0.92
2:F:237:VAL:HG22	2:F:238:SER:H	1.35	0.92
1:D:119:LYS:O	1:D:120:ILE:HG13	1.70	0.91
1:A:94:GLN:NE2	1:A:125:ASP:H	1.68	0.91
1:B:48:ASP:O	1:B:82:THR:HB	1.68	0.91
2:E:113:ARG:HB3	2:E:156:HIS:HE1	1.37	0.89
2:E:113:ARG:HD3	2:E:156:HIS:CE1	2.07	0.89
1:A:30:ASN:O	1:A:65:ARG:HG3	1.72	0.89
2:E:159:LEU:HD12	2:E:160:SER:N	1.88	0.89
2:E:226:THR:HG23	2:E:227:GLN:N	1.88	0.89
1:A:31:PHE:HE1	1:A:33:THR:HG23	1.38	0.88
1:A:94:GLN:HE21	1:A:124:LYS:HA	1.39	0.88
2:E:144:THR:HA	2:E:197:ARG:HA	1.56	0.88
2:E:186:ASN:C	2:E:188:SER:H	1.79	0.88
1:B:69:VAL:HG21	1:B:90:ILE:HD13	1.54	0.87
2:E:106:GLN:O	2:E:107:TYR:HB2	1.74	0.87
1:C:69:VAL:CG2	1:C:90:ILE:HG23	2.05	0.86
1:A:28:ARG:HD3	1:A:28:ARG:H	1.40	0.86
1:D:45:ARG:HG2	1:D:45:ARG:HH11	1.39	0.86
1:A:78:LEU:HD13	2:E:52:GLY:HA3	1.58	0.85
2:E:23:CYS:SG	2:E:32:MET:HE1	2.15	0.85
2:E:153:TYR:HB3	2:E:154:PRO:HD3	1.58	0.84
2:E:12:ILE:H	2:E:12:ILE:CD1	1.90	0.84
2:F:12:ILE:HA	2:F:115:THR:HG22	1.57	0.84
2:E:214:VAL:HB	2:E:237:VAL:HG23	1.60	0.84
2:E:158:GLU:HB3	2:E:215:GLN:CB	2.08	0.83
1:D:167:HIS:HE1	1:D:169:GLN:HG3	1.41	0.83
2:E:64:LYS:HE3	2:E:64:LYS:HA	1.57	0.83
1:D:13:LEU:HD13	1:D:147:TYR:CD1	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD22	2:E:52:GLY:HA2	1.61	0.83
2:E:136:GLU:O	2:E:140:THR:HB	1.79	0.83
2:E:144:THR:HB	2:E:197:ARG:HB2	1.61	0.83
1:C:102:LEU:HD21	1:C:196:MET:HE1	1.61	0.82
2:E:7:HIS:N	2:E:8:PRO:HD3	1.89	0.82
2:E:208:ASN:C	2:E:208:ASN:HD22	1.87	0.82
1:B:197:LYS:HG3	1:D:163:LYS:O	1.80	0.82
2:E:219:LEU:HG	2:E:233:VAL:HA	1.60	0.82
1:A:77:ILE:O	1:A:78:LEU:HD12	1.80	0.81
1:A:77:ILE:C	1:A:78:LEU:HD12	2.05	0.81
2:F:47:ALA:HB3	2:F:67:ILE:HG21	1.60	0.81
2:E:227:GLN:HG2	2:E:231:LYS:HD2	1.63	0.81
2:F:77:LEU:O	2:F:77:LEU:HD23	1.78	0.81
1:D:29:VAL:O	1:D:65:ARG:HA	1.81	0.81
2:F:86:ASP:CB	2:F:115:THR:HA	2.06	0.81
1:A:79:ASN:C	1:A:81:HIS:H	1.88	0.80
1:C:6:ILE:HG23	1:C:7:SER:N	1.96	0.80
1:C:156:GLY:HA2	1:C:157:ARG:HH21	1.45	0.80
2:E:64:LYS:O	2:E:80:THR:HG23	1.81	0.80
1:A:117:ASN:O	1:A:118:ASN:HB2	1.80	0.80
2:F:36:ARG:HG2	2:F:37:GLN:N	1.90	0.80
1:B:157:ARG:HH11	1:B:157:ARG:HG2	1.47	0.79
1:B:64:LYS:NZ	1:B:65:ARG:HB3	1.97	0.79
1:B:190:ASP:OD1	1:B:192:ARG:HG2	1.83	0.79
1:D:178:GLU:O	1:D:180:THR:N	2.16	0.79
1:D:27:CYS:O	1:D:68:HIS:HA	1.81	0.79
2:E:120:LEU:HD22	2:E:221:GLU:O	1.83	0.78
2:E:219:LEU:HD22	2:E:220:SER:N	1.97	0.78
2:E:125:PRO:HB3	2:E:152:PHE:HB3	1.65	0.78
1:B:9:VAL:HG22	1:B:175:SER:HB3	1.66	0.77
1:C:6:ILE:O	1:C:9:VAL:HB	1.84	0.77
2:E:159:LEU:CD1	2:E:160:SER:H	1.96	0.77
1:B:69:VAL:HG21	1:B:90:ILE:CD1	2.14	0.77
1:B:78:LEU:HB2	2:F:52:GLY:HA2	1.67	0.77
1:C:126:ILE:HG23	1:C:193:ILE:HD12	1.65	0.77
1:C:14:LEU:HD23	1:C:14:LEU:O	1.85	0.77
2:E:79:VAL:HG13	2:E:80:THR:N	1.98	0.77
2:E:200:ALA:O	2:E:204:GLN:HG2	1.85	0.77
2:F:10:ARG:HH12	2:F:215:GLN:CB	1.98	0.77
2:F:130:PHE:N	2:F:146:VAL:O	2.18	0.77
2:F:206:PRO:O	2:F:208:ASN:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:206:PRO:C	2:E:208:ASN:H	1.92	0.76
1:D:5:ASP:O	1:D:7:SER:N	2.18	0.76
2:F:21:ILE:HD12	2:F:77:LEU:HD22	1.68	0.76
1:B:55:MET:HB3	1:B:59:ALA:CB	2.16	0.76
1:D:129:PHE:CZ	1:D:194:ILE:HD11	2.21	0.76
2:F:126:GLU:HA	2:F:126:GLU:OE1	1.83	0.76
1:A:102:LEU:HD12	1:A:120:ILE:HG22	1.67	0.76
2:E:122:ASN:O	2:E:123:PHE:HB2	1.86	0.75
2:E:231:LYS:O	2:E:231:LYS:HD3	1.86	0.75
1:B:10:LYS:HZ3	1:B:151:SER:HB3	1.52	0.75
2:E:201:THR:O	2:E:202:PHE:HB3	1.85	0.75
1:D:3:LYS:HD2	1:D:4:LYS:H	1.51	0.75
2:E:129:VAL:HG23	2:E:239:ALA:HB3	1.67	0.75
1:C:88:GLY:O	1:C:90:ILE:HG12	1.87	0.75
2:E:166:LYS:HD2	2:E:166:LYS:N	2.02	0.74
1:A:69:VAL:CG2	1:A:90:ILE:HG23	2.14	0.74
2:F:129:VAL:C	2:F:130:PHE:HA	2.12	0.74
1:C:43:LYS:HE3	1:C:44:TYR:CE2	2.22	0.74
1:B:28:ARG:HG3	1:B:66:ASP:OD1	1.88	0.74
1:A:79:ASN:HB2	2:E:30:THR:HG21	1.69	0.73
2:E:40:LYS:HG3	2:E:41:GLN:H	1.51	0.73
1:B:90:ILE:O	1:B:90:ILE:HG13	1.87	0.73
1:B:160:ILE:HG23	1:B:199:PHE:HE1	1.53	0.73
1:D:129:PHE:HA	1:D:132:ILE:HG22	1.71	0.73
1:C:65:ARG:HG3	1:C:66:ASP:OD2	1.88	0.73
1:D:69:VAL:HG21	1:D:90:ILE:CG2	2.17	0.73
2:E:144:THR:HA	2:E:197:ARG:CA	2.18	0.73
2:E:102:THR:O	2:E:103:ASP:HB3	1.88	0.73
2:E:113:ARG:HD3	2:E:156:HIS:ND1	2.03	0.73
1:C:157:ARG:HE	1:C:157:ARG:N	1.86	0.72
1:A:108:ILE:HG23	1:A:206:LEU:HB2	1.71	0.72
2:E:52:GLY:O	2:E:69:HIS:ND1	2.23	0.72
1:A:79:ASN:O	1:A:81:HIS:N	2.23	0.72
1:A:22:TYR:O	1:A:72:PHE:HA	1.89	0.72
2:F:19:VAL:HB	2:F:79:VAL:CG2	2.18	0.72
2:F:86:ASP:O	2:F:87:SER:HB3	1.88	0.72
1:C:21:PRO:HB3	1:C:74:LEU:HD23	1.69	0.72
1:C:124:LYS:HB2	1:C:127:VAL:HG23	1.72	0.72
2:F:6:GLN:OE1	2:F:91:ILE:HA	1.88	0.72
2:F:44:MET:C	2:F:45:LEU:HD22	2.15	0.71
2:F:12:ILE:HA	2:F:115:THR:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:SER:O	1:B:201:HIS:HB3	1.90	0.71
2:E:219:LEU:HG	2:E:233:VAL:C	2.16	0.71
2:E:14:LYS:HB2	2:E:14:LYS:NZ	2.05	0.71
2:E:66:LEU:HB3	2:E:78:THR:HG23	1.72	0.71
1:A:99:ASN:OD1	1:A:121:ILE:HG21	1.90	0.71
1:C:45:ARG:HG3	1:C:45:ARG:HH11	1.54	0.71
1:D:6:ILE:HD11	1:D:173:PHE:CD2	2.25	0.71
2:E:159:LEU:CD1	2:E:160:SER:N	2.54	0.71
1:B:27:CYS:HB3	1:B:40:ASP:O	1.91	0.71
2:E:26:LEU:HD23	2:E:27:ASP:N	2.05	0.71
2:E:226:THR:HG23	2:E:227:GLN:HG3	1.72	0.71
1:A:28:ARG:HG2	1:A:40:ASP:CB	2.20	0.71
2:E:64:LYS:HB3	2:E:80:THR:HG21	1.73	0.71
1:A:64:LYS:O	1:A:65:ARG:O	2.09	0.71
1:B:10:LYS:NZ	1:B:151:SER:HB3	2.05	0.71
1:C:7:SER:C	1:C:9:VAL:H	1.98	0.70
2:E:226:THR:HG23	2:E:227:GLN:H	1.55	0.70
1:A:180:THR:HG22	2:E:54:ALA:CB	2.15	0.70
2:F:9:SER:O	2:F:112:THR:HG23	1.92	0.70
1:D:111:GLU:O	1:D:112:SER:CB	2.38	0.70
2:F:21:ILE:HD12	2:F:77:LEU:CD2	2.21	0.70
2:E:52(A):SER:O	2:E:53:LYS:C	2.33	0.70
1:D:128:THR:HG23	1:D:131:GLU:H	1.56	0.70
1:D:159:GLU:HA	1:D:168:GLU:O	1.91	0.70
1:A:56:SER:H	1:A:189:LYS:HG2	1.57	0.70
2:F:12:ILE:HD12	2:F:233:VAL:HA	1.74	0.70
2:E:63:ASP:O	2:E:65:PHE:N	2.23	0.69
1:B:11:SER:HA	1:B:14:LEU:HD22	1.74	0.69
1:B:154:VAL:HG13	1:B:155:SER:H	1.56	0.69
2:E:20:LYS:H	2:E:20:LYS:HD2	1.57	0.69
2:E:173:SER:HB3	2:E:195:ARG:HD3	1.74	0.69
1:A:69:VAL:HG21	1:A:90:ILE:CG2	2.20	0.69
2:E:14:LYS:HB2	2:E:14:LYS:HZ2	1.58	0.69
1:A:30:ASN:C	1:A:30:ASN:HD22	1.99	0.69
1:A:180:THR:HB	2:E:53:LYS:O	1.93	0.69
1:B:51:ILE:CD1	1:B:84:GLU:HB2	2.23	0.69
1:D:42:GLN:HG2	1:D:46:GLY:O	1.93	0.69
2:F:115:THR:HG21	2:F:217:TYR:O	1.92	0.69
1:C:17:TYR:O	1:C:19:ILE:N	2.26	0.69
2:E:159:LEU:HD22	2:E:174:THR:HG21	1.75	0.69
1:B:102:LEU:HD21	1:B:122:LEU:HD23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:120:LEU:HD13	2:E:221:GLU:CB	2.24	0.68
2:E:219:LEU:HG	2:E:233:VAL:CA	2.23	0.68
1:A:76:TYR:CD1	1:A:77:ILE:HG12	2.28	0.68
2:E:64:LYS:HB3	2:E:80:THR:CG2	2.23	0.68
1:C:145:LYS:HB3	1:C:148:ASP:OD1	1.94	0.68
1:D:30:ASN:O	1:D:31:PHE:HB3	1.94	0.68
1:D:71:VAL:HG22	1:D:90:ILE:CD1	2.24	0.68
2:E:40:LYS:HG3	2:E:41:GLN:N	2.08	0.68
2:E:88:SER:OG	2:E:89:PHE:N	2.25	0.68
2:F:74:LEU:HG	2:F:75:SER:N	2.09	0.68
1:C:157:ARG:HE	1:C:157:ARG:H	1.42	0.67
2:E:52:GLY:O	2:E:52(A):SER:HB2	1.92	0.67
1:D:36:THR:HG22	1:D:54:GLU:HA	1.76	0.67
1:D:71:VAL:HG22	1:D:90:ILE:HD13	1.75	0.67
1:B:154:VAL:HG13	1:B:155:SER:N	2.09	0.67
1:A:79:ASN:O	1:A:79:ASN:ND2	2.28	0.67
1:A:166:LYS:HD3	1:A:167:HIS:N	2.10	0.67
1:D:77:ILE:HG12	1:D:78:LEU:N	2.10	0.67
2:E:127:VAL:HG21	2:E:214:VAL:HG21	1.77	0.67
2:E:186:ASN:C	2:E:188:SER:N	2.49	0.67
1:C:69:VAL:HG21	1:C:90:ILE:CG2	2.22	0.66
2:E:60:VAL:HG22	2:E:60:VAL:O	1.93	0.66
2:F:237:VAL:HG22	2:F:238:SER:N	2.10	0.66
1:A:136:ILE:O	1:A:139:TYR:O	2.13	0.66
1:A:48:ASP:O	1:A:82:THR:CG2	2.44	0.66
1:A:56:SER:N	1:A:189:LYS:HG2	2.10	0.66
1:B:64:LYS:HZ3	1:B:65:ARG:HB3	1.60	0.66
2:F:207:ARG:O	2:F:207:ARG:HG2	1.95	0.66
1:C:21:PRO:HB3	1:C:74:LEU:CD2	2.25	0.66
1:C:96:ASN:O	1:C:98:VAL:HG13	1.96	0.66
1:A:32:SER:HB2	1:A:37:LEU:HD12	1.78	0.66
1:A:166:LYS:HD3	1:A:166:LYS:C	2.19	0.66
1:D:111:GLU:O	1:D:112:SER:HB3	1.94	0.66
2:E:142:LYS:HD2	2:E:197:ARG:HH11	1.60	0.66
2:F:18:SER:HA	2:F:79:VAL:O	1.96	0.66
2:F:147:CYS:HG	2:F:194:SER:HG	1.34	0.66
2:F:86:ASP:OD1	2:F:116:VAL:HB	1.95	0.66
2:F:38:PHE:HA	2:F:88:SER:OG	1.96	0.65
1:B:31:PHE:O	1:B:38:ASN:HB3	1.96	0.65
1:C:41:THR:HG21	1:C:51:ILE:HG12	1.77	0.65
1:C:122:LEU:HD12	1:C:196:MET:CE	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:SER:HB3	2:E:83:HIS:ND1	2.11	0.65
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.61	0.65
1:C:24:TYR:HE2	1:C:51:ILE:HD11	1.61	0.65
1:D:42:GLN:O	1:D:43:LYS:HG2	1.96	0.65
2:F:129:VAL:CG1	2:F:239:ALA:HB1	2.26	0.65
1:C:73:GLY:HA2	1:C:130:GLN:OE1	1.95	0.65
1:A:184:ILE:C	1:A:186:ALA:H	2.04	0.65
1:B:124:LYS:HB2	1:B:127:VAL:CG2	2.23	0.65
2:E:154:PRO:O	2:E:156:HIS:N	2.30	0.65
1:A:180:THR:CG2	2:E:54:ALA:HB2	2.17	0.65
1:B:201:HIS:HB3	1:D:103:LEU:CD1	2.26	0.65
1:D:6:ILE:HG13	1:D:10:LYS:HD2	1.78	0.65
1:B:78:LEU:H	2:F:52:GLY:HA3	1.59	0.65
2:E:113:ARG:HB3	2:E:156:HIS:CE1	2.27	0.65
2:E:158:GLU:CB	2:E:215:GLN:HB3	2.26	0.65
2:F:124:PRO:N	2:F:125:PRO:HD3	2.12	0.65
1:B:102:LEU:HD11	1:B:122:LEU:CD2	2.27	0.64
1:D:3:LYS:HD2	1:D:4:LYS:N	2.11	0.64
1:C:141:MET:HE3	1:C:147:TYR:CD2	2.21	0.64
2:F:50:ALA:HB3	2:F:53:LYS:HB2	1.79	0.64
1:B:69:VAL:CG2	1:B:70:ASP:N	2.61	0.64
1:B:101:LYS:HB3	1:B:118:ASN:OD1	1.97	0.64
1:D:64:LYS:HG2	1:D:65:ARG:HG2	1.78	0.64
2:F:86:ASP:HB3	2:F:115:THR:CA	2.09	0.64
1:A:184:ILE:O	1:A:187:LYS:HG2	1.97	0.64
1:A:81:HIS:HA	2:E:28:GLN:HE21	1.61	0.64
1:A:114:GLN:CD	1:A:115:ASN:H	2.06	0.64
1:C:126:ILE:CG2	1:C:193:ILE:HD12	2.27	0.64
1:D:116:LEU:O	1:D:119:LYS:HB2	1.98	0.64
2:E:22:GLU:HA	2:E:76:THR:HG22	1.79	0.64
2:F:30:THR:HG23	2:F:31:THR:N	2.09	0.64
2:F:129:VAL:HG13	2:F:239:ALA:HB1	1.79	0.64
1:C:6:ILE:C	1:C:6:ILE:HD13	2.22	0.64
1:B:100:HIS:CD2	1:B:196:MET:HG3	2.33	0.63
2:F:192:LEU:HD12	2:F:192:LEU:N	2.13	0.63
2:E:57:GLU:OE2	2:E:63:ASP:CB	2.35	0.63
2:E:219:LEU:CG	2:E:233:VAL:HA	2.27	0.63
1:C:102:LEU:HD11	1:C:122:LEU:HG	1.79	0.63
2:E:132:PRO:HD2	2:E:203:TRP:CZ2	2.33	0.63
2:F:194:SER:O	2:F:195:ARG:HB3	1.98	0.63
1:A:75:PHE:CD1	1:A:75:PHE:C	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG23	1:D:91:THR:O	1.99	0.63
2:E:153:TYR:O	2:E:154:PRO:C	2.40	0.63
1:A:8:ASN:O	1:A:9:VAL:HG23	1.99	0.63
1:B:180:THR:HG21	2:F:53:LYS:CE	2.29	0.63
1:A:55:MET:SD	1:A:60:SER:HB3	2.39	0.63
1:C:63:PHE:C	1:C:64:LYS:HG3	2.24	0.62
2:E:216:PHE:CB	2:E:235:GLN:O	2.47	0.62
1:B:201:HIS:HB3	1:D:103:LEU:HD11	1.80	0.62
1:B:156:GLY:O	1:B:172:LEU:HB2	1.99	0.62
2:E:165:GLY:C	2:E:166:LYS:HD2	2.24	0.62
2:E:180:LYS:HE3	2:E:188:SER:OG	1.98	0.62
1:B:74:LEU:HB2	1:B:185:PHE:CE2	2.34	0.62
1:C:94:GLN:HE22	1:C:125:ASP:H	1.48	0.62
2:E:71:SER:C	2:E:73:THR:H	2.08	0.62
1:A:70:ASP:OD2	1:A:93:ALA:HA	1.99	0.62
1:A:130:GLN:HG3	1:A:188:TYR:CD2	2.34	0.62
1:D:167:HIS:CE1	1:D:169:GLN:HG3	2.30	0.62
1:A:55:MET:HG3	1:A:60:SER:HB3	1.81	0.62
1:A:114:GLN:NE2	1:A:115:ASN:H	1.98	0.62
1:A:139:TYR:O	1:A:140:LEU:CB	2.48	0.62
1:B:63:PHE:CE2	1:B:90:ILE:HD11	2.34	0.62
1:D:129:PHE:O	1:D:132:ILE:HG22	2.00	0.62
2:E:62:LYS:C	2:E:64:LYS:H	2.06	0.62
1:A:190:ASP:O	1:A:191:ASN:C	2.42	0.62
1:B:74:LEU:O	1:B:86:ILE:HG22	2.00	0.62
2:E:58:GLN:HG3	2:E:59:GLY:H	1.63	0.62
2:F:127:VAL:HB	2:F:149:ALA:HA	1.80	0.61
1:A:124:LYS:HB2	1:A:127:VAL:HG23	1.82	0.61
2:E:227:GLN:HE21	2:E:231:LYS:NZ	1.97	0.61
2:F:114:LEU:O	2:F:115:THR:HB	1.99	0.61
1:A:10:LYS:NZ	1:A:151:SER:HB3	2.14	0.61
2:E:140:THR:HG22	2:E:142:LYS:H	1.64	0.61
1:A:78:LEU:HD13	2:E:52:GLY:CA	2.29	0.61
1:D:51:ILE:HD13	1:D:84:GLU:HB2	1.82	0.61
2:E:79:VAL:CG1	2:E:80:THR:H	1.99	0.61
2:E:215:GLN:HG2	2:E:217:TYR:CE2	2.36	0.61
1:A:157:ARG:HB2	1:A:170:ILE:O	2.01	0.61
1:B:106:LEU:HD23	1:B:107:PHE:N	2.15	0.61
1:C:9:VAL:C	1:C:11:SER:H	2.09	0.61
2:E:18:SER:CA	2:E:80:THR:O	2.46	0.61
1:D:11:SER:C	1:D:13:LEU:H	2.06	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:SER:O	2:E:99:GLY:C	2.43	0.61
1:D:29:VAL:HB	1:D:64:LYS:O	2.00	0.61
1:D:45:ARG:HB3	1:D:49:TYR:CG	2.36	0.61
1:D:45:ARG:HH11	1:D:45:ARG:CG	2.12	0.61
1:D:81:HIS:ND1	1:D:81:HIS:C	2.58	0.61
2:E:163:VAL:HG22	2:E:210:PHE:CE1	2.36	0.61
1:B:78:LEU:HB2	2:F:52:GLY:CA	2.31	0.61
1:D:24:TYR:OH	1:D:45:ARG:NH1	2.30	0.61
2:E:64:LYS:O	2:E:80:THR:CG2	2.49	0.61
2:F:41:GLN:O	2:F:42:SER:CB	2.49	0.61
1:C:41:THR:HG21	1:C:51:ILE:CG1	2.31	0.60
1:C:49:TYR:CE1	1:C:82:THR:HG22	2.37	0.60
1:C:128:THR:HG23	1:C:131:GLU:H	1.66	0.60
2:F:27(A):PHE:CG	2:F:28:GLN:N	2.68	0.60
1:B:22:TYR:O	1:B:72:PHE:HA	2.01	0.60
2:E:79:VAL:O	2:E:80:THR:HG23	2.00	0.60
2:F:187:ASP:O	2:F:188:SER:HB2	2.01	0.60
2:E:65:PHE:CE1	2:E:79:VAL:HG23	2.36	0.60
2:F:86:ASP:O	2:F:87:SER:CB	2.49	0.60
1:A:9:VAL:C	1:A:11:SER:N	2.57	0.60
1:A:191:ASN:O	1:A:191:ASN:ND2	2.31	0.60
2:E:26:LEU:O	2:E:27:ASP:C	2.44	0.60
2:E:117:LEU:HD11	2:E:154:PRO:HG3	1.82	0.60
2:E:227:GLN:HE21	2:E:231:LYS:HZ3	1.49	0.60
1:A:6:ILE:HG12	1:A:154:VAL:HG23	1.84	0.60
1:A:154:VAL:HG12	1:A:207:GLU:O	2.02	0.60
1:D:77:ILE:HG12	1:D:78:LEU:H	1.66	0.60
2:E:145:LEU:HD21	2:E:210:PHE:CD2	2.36	0.60
2:E:182:GLN:O	2:E:185:LEU:HD21	2.02	0.60
2:E:210:PHE:HB2	2:E:241:ALA:O	2.02	0.60
1:C:164:ASP:OD1	1:C:166:LYS:HE3	2.01	0.60
1:D:124:LYS:HB2	1:D:127:VAL:HG22	1.84	0.60
2:E:127:VAL:CG2	2:E:214:VAL:HG21	2.32	0.60
1:C:21:PRO:HG3	1:C:134:PHE:CE2	2.37	0.59
1:D:72:PHE:CD1	1:D:72:PHE:C	2.80	0.59
1:D:140:LEU:HD21	1:D:204:ILE:HD13	1.85	0.59
2:E:15:SER:CA	2:E:82:ALA:O	2.42	0.59
2:E:206:PRO:C	2:E:208:ASN:N	2.59	0.59
2:E:215:GLN:HG3	2:E:215:GLN:O	2.00	0.59
1:A:108:ILE:HG23	1:A:206:LEU:CB	2.32	0.59
1:B:55:MET:HB3	1:B:59:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:O	1:B:204:ILE:HG12	2.03	0.59
1:C:157:ARG:NH2	1:C:207:GLU:OE2	2.36	0.59
1:B:72:PHE:CD1	1:B:72:PHE:C	2.79	0.59
1:B:180:THR:HG21	2:F:53:LYS:HE2	1.83	0.59
1:C:80:SER:O	1:C:81:HIS:HB2	2.01	0.59
1:C:129:PHE:HE2	1:C:160:ILE:HG13	1.67	0.59
1:D:158:ILE:HD11	1:D:172:LEU:HD21	1.83	0.59
2:F:50:ALA:O	2:F:51:GLU:C	2.45	0.59
1:B:103:LEU:CD1	1:D:201:HIS:HB3	2.32	0.59
1:B:184:ILE:N	1:B:184:ILE:HD12	2.17	0.59
1:D:163:LYS:HD2	1:D:200:SER:HB2	1.84	0.59
2:E:45:LEU:HD23	2:E:58:GLN:HG2	1.84	0.59
2:E:219:LEU:CD1	2:E:233:VAL:HA	2.32	0.59
1:A:191:ASN:C	1:A:191:ASN:HD22	2.09	0.59
1:B:201:HIS:CG	1:D:103:LEU:HD11	2.36	0.59
1:C:22:TYR:CE2	1:C:75:PHE:HB3	2.37	0.59
2:E:22:GLU:HG2	2:E:76:THR:HG22	1.84	0.59
2:E:129:VAL:HG23	2:E:239:ALA:CB	2.33	0.59
2:F:61:GLU:O	2:F:62:LYS:HE2	2.03	0.59
1:B:19:ILE:HG12	1:B:20:THR:N	2.18	0.59
1:C:6:ILE:CG2	1:C:7:SER:H	2.10	0.59
2:E:22:GLU:HG2	2:E:76:THR:CG2	2.32	0.59
2:E:153:TYR:HB3	2:E:154:PRO:CD	2.28	0.59
2:F:17:THR:H	2:F:81:SER:CB	2.15	0.59
1:B:55:MET:HB3	1:B:59:ALA:HB3	1.85	0.58
1:C:49:TYR:CZ	1:C:82:THR:HG22	2.37	0.58
1:C:124:LYS:NZ	1:C:131:GLU:OE1	2.32	0.58
1:B:60:SER:C	1:B:62:LYS:N	2.60	0.58
1:B:78:LEU:HD12	2:F:52:GLY:O	2.03	0.58
1:B:163:LYS:NZ	1:D:199:PHE:O	2.29	0.58
1:C:50:TYR:CZ	1:C:83:GLY:HA3	2.38	0.58
1:C:158:ILE:HB	1:C:170:ILE:HB	1.85	0.58
1:A:79:ASN:HB2	2:E:30:THR:CG2	2.34	0.58
1:A:22:TYR:CE2	1:A:84:GLU:HB3	2.39	0.58
1:B:4:LYS:NZ	1:B:4:LYS:HB3	2.19	0.58
1:C:27:CYS:O	1:C:69:VAL:HG12	2.04	0.58
1:D:6:ILE:HG13	1:D:10:LYS:HG3	1.86	0.58
1:D:9:VAL:O	1:D:13:LEU:HD12	2.03	0.58
1:D:13:LEU:HD13	1:D:147:TYR:CE1	2.38	0.58
2:E:25:SER:O	2:E:73:THR:HG23	2.03	0.58
2:F:36:ARG:CG	2:F:37:GLN:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:N	1:C:157:ARG:NE	2.51	0.58
2:E:87:SER:OG	2:E:116:VAL:HG22	2.04	0.58
1:D:184:ILE:HD11	1:D:187:LYS:NZ	2.18	0.58
1:C:108:ILE:O	1:C:110:GLY:N	2.35	0.58
2:E:97:GLY:O	2:E:98:SER:CB	2.52	0.58
1:B:42:GLN:HA	1:B:46:GLY:O	2.02	0.58
1:B:4:LYS:HB3	1:B:4:LYS:HZ3	1.69	0.57
1:A:168:GLU:CD	1:A:192:ARG:NH1	2.62	0.57
1:C:77:ILE:HG12	1:C:78:LEU:N	2.20	0.57
1:A:81:HIS:CG	1:A:81:HIS:O	2.58	0.57
1:B:154:VAL:HG12	1:B:207:GLU:O	2.03	0.57
2:E:95:LEU:HD23	2:E:106:GLN:HB2	1.86	0.57
2:E:10:ARG:C	2:E:11:VAL:HG23	2.29	0.57
1:A:28:ARG:HD3	1:A:28:ARG:N	2.15	0.57
1:B:103:LEU:HD11	1:D:201:HIS:HB3	1.87	0.57
2:E:54:ALA:C	2:E:55:THR:HG22	2.29	0.57
2:E:201:THR:O	2:E:202:PHE:CB	2.51	0.57
1:A:102:LEU:HD11	1:A:122:LEU:HG	1.87	0.57
1:C:117:ASN:O	1:C:118:ASN:HB2	2.04	0.57
2:E:219:LEU:HD13	2:E:220:SER:HB2	1.87	0.57
2:F:44:MET:O	2:F:45:LEU:HD13	2.04	0.57
2:F:71:SER:OG	2:F:72:LEU:HD23	2.04	0.57
1:D:45:ARG:HG2	1:D:45:ARG:NH1	2.14	0.57
1:D:129:PHE:CA	1:D:132:ILE:HG22	2.35	0.57
2:E:68:ASN:N	2:E:68:ASN:HD22	2.03	0.57
2:E:127:VAL:HG21	2:E:214:VAL:CG2	2.34	0.57
1:A:122:LEU:HD13	1:A:127:VAL:HG11	1.86	0.57
1:A:139:TYR:O	1:A:140:LEU:HG	2.05	0.57
1:B:76:TYR:CA	1:B:181:ARG:HB3	2.29	0.57
2:E:64:LYS:HD2	2:E:64:LYS:N	2.20	0.57
2:F:192:LEU:HD12	2:F:192:LEU:H	1.67	0.57
1:A:104:GLY:H	1:A:117:ASN:ND2	2.03	0.57
1:C:101:LYS:HD3	1:C:118:ASN:OD1	2.05	0.57
2:F:69:HIS:HA	2:F:75:SER:HB3	1.87	0.56
1:B:36:THR:HA	1:B:53:SER:O	2.05	0.56
1:C:39:ILE:HG12	1:C:69:VAL:HG11	1.86	0.56
2:F:5:SER:O	2:F:23:CYS:HA	2.05	0.56
1:B:65:ARG:O	1:B:66:ASP:C	2.47	0.56
1:C:51:ILE:HD13	1:C:84:GLU:HB2	1.87	0.56
1:C:136:ILE:O	1:C:139:TYR:HB3	2.05	0.56
1:D:120:ILE:HG22	1:D:120:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:LEU:N	2:E:43:LEU:HD23	2.20	0.56
2:F:236:ILE:HG12	2:F:237:VAL:N	2.20	0.56
1:A:54:GLU:OE2	1:A:189:LYS:HE3	2.06	0.56
2:E:43:LEU:CD1	2:E:108:PHE:HZ	2.03	0.56
2:E:73:THR:HG22	2:E:73:THR:O	2.05	0.56
2:E:208:ASN:C	2:E:208:ASN:ND2	2.57	0.56
2:E:209:HIS:NE2	2:E:211:ARG:HB3	2.19	0.56
1:A:13:LEU:O	1:A:16:ALA:N	2.38	0.56
1:B:36:THR:HG22	1:B:54:GLU:HA	1.86	0.56
2:E:125:PRO:HG2	2:E:237:VAL:HG21	1.88	0.56
2:E:143:ALA:O	2:E:197:ARG:HA	2.05	0.56
2:F:36:ARG:NH1	2:F:65:PHE:HE1	2.04	0.56
2:F:238:SER:OG	2:F:239:ALA:N	2.39	0.56
1:D:39:ILE:CD1	1:D:90:ILE:HD12	2.35	0.56
2:E:27(A):PHE:HE1	2:E:94:ALA:CB	2.19	0.56
1:D:129:PHE:CE2	1:D:194:ILE:HD11	2.41	0.56
2:E:10:ARG:HG3	2:E:11:VAL:HG23	1.88	0.56
2:E:227:GLN:CG	2:E:231:LYS:HD2	2.36	0.56
1:D:28:ARG:HB3	1:D:68:HIS:CE1	2.40	0.56
2:E:10:ARG:HD2	2:E:217:TYR:HB3	1.88	0.56
2:F:147:CYS:SG	2:F:148:LEU:N	2.79	0.56
1:B:70:ASP:CG	1:B:93:ALA:HA	2.31	0.55
1:C:18:THR:HG22	1:C:18:THR:O	2.06	0.55
2:E:83:HIS:O	2:E:84:PRO:C	2.49	0.55
1:A:14:LEU:O	1:A:14:LEU:HD23	2.06	0.55
1:A:55:MET:CG	1:A:60:SER:HB3	2.37	0.55
2:E:64:LYS:HA	2:E:64:LYS:CE	2.28	0.55
2:E:87:SER:HA	2:E:114:LEU:O	2.07	0.55
1:B:78:LEU:HD12	2:F:52:GLY:C	2.31	0.55
1:C:29:VAL:HG11	1:C:37:LEU:HD11	1.87	0.55
1:D:3:LYS:CD	1:D:4:LYS:H	2.19	0.55
1:D:94:GLN:NE2	1:D:125:ASP:H	2.03	0.55
2:E:68:ASN:ND2	2:E:76:THR:OG1	2.32	0.55
2:F:234:THR:O	2:F:235:GLN:CB	2.54	0.55
1:B:37:LEU:HD23	1:B:90:ILE:HG12	1.89	0.55
1:B:201:HIS:CB	1:D:103:LEU:HD11	2.36	0.55
1:A:13:LEU:O	1:A:14:LEU:C	2.49	0.55
1:B:37:LEU:HB2	1:B:55:MET:HE2	1.89	0.55
2:E:118:GLU:HG3	2:E:119:ASP:N	2.22	0.55
1:D:72:PHE:CE2	1:D:131:GLU:HG3	2.42	0.55
2:F:20:LYS:C	2:F:21:ILE:HG13	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:HIS:HA	2:F:75:SER:CB	2.36	0.55
1:A:79:ASN:HB2	2:E:30:THR:CB	2.37	0.55
1:B:130:GLN:O	1:B:133:ASP:HB3	2.06	0.55
1:B:168:GLU:CD	1:B:192:ARG:HH12	2.15	0.55
1:B:60:SER:O	1:B:62:LYS:N	2.39	0.54
1:B:107:PHE:CD2	1:B:205:TYR:CE1	2.95	0.54
1:B:164:ASP:N	1:B:164:ASP:OD1	2.40	0.54
1:C:21:PRO:HG3	1:C:134:PHE:HE2	1.71	0.54
1:D:10:LYS:HB3	1:D:147:TYR:O	2.07	0.54
1:D:5:ASP:C	1:D:7:SER:H	2.15	0.54
1:A:73:GLY:HA2	1:A:130:GLN:OE1	2.06	0.54
1:B:29:VAL:HA	1:B:39:ILE:HA	1.89	0.54
1:B:90:ILE:O	1:B:90:ILE:CG1	2.54	0.54
2:E:142:LYS:HD3	2:E:197:ARG:HE	1.72	0.54
2:F:71:SER:C	2:F:73:THR:N	2.63	0.54
2:F:237:VAL:HG13	2:F:238:SER:N	2.21	0.54
1:A:139:TYR:O	1:A:140:LEU:HB2	2.06	0.54
1:D:6:ILE:CG1	1:D:10:LYS:HD2	2.38	0.54
2:E:50:ALA:O	2:E:52:GLY:N	2.41	0.54
2:E:71:SER:C	2:E:73:THR:N	2.63	0.54
2:F:207:ARG:O	2:F:208:ASN:O	2.26	0.54
1:B:65:ARG:HG3	1:B:66:ASP:H	1.71	0.54
1:C:132:ILE:O	1:C:133:ASP:C	2.50	0.54
1:D:6:ILE:HG13	1:D:10:LYS:CD	2.37	0.54
1:D:39:ILE:HD13	1:D:69:VAL:HG11	1.89	0.54
1:B:67:ASP:O	1:B:69:VAL:HG12	2.08	0.54
1:C:19:ILE:HD11	1:C:75:PHE:CD2	2.43	0.54
2:E:62:LYS:C	2:E:64:LYS:N	2.65	0.54
2:E:153:TYR:O	2:E:155:ASP:N	2.41	0.54
2:F:233:VAL:HG12	2:F:234:THR:HG23	1.87	0.54
1:B:8:ASN:N	1:B:8:ASN:HD22	2.05	0.54
2:E:27(A):PHE:O	2:E:28:GLN:CB	2.55	0.54
1:A:56:SER:HA	1:A:189:LYS:HE2	1.90	0.54
1:D:9:VAL:C	1:D:11:SER:H	2.14	0.54
2:E:20:LYS:HD2	2:E:20:LYS:N	2.22	0.54
1:D:11:SER:C	1:D:13:LEU:N	2.66	0.53
2:E:223:ASP:O	2:E:224:GLU:HB2	2.07	0.53
1:B:150:THR:O	1:B:151:SER:HB2	2.09	0.53
1:B:181:ARG:HH11	2:F:52(A):SER:CB	2.21	0.53
1:C:106:LEU:HD11	1:C:144:TYR:CE2	2.43	0.53
1:C:129:PHE:CE2	1:C:160:ILE:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:ILE:HG12	2:F:217:TYR:O	2.08	0.53
1:A:180:THR:HG21	2:E:53:LYS:NZ	2.24	0.53
1:B:157:ARG:HH11	1:B:157:ARG:CG	2.17	0.53
1:D:45:ARG:NH2	1:D:84:GLU:OE2	2.40	0.53
1:D:75:PHE:CD1	1:D:75:PHE:C	2.87	0.53
1:A:3:LYS:O	1:A:5:ASP:OD2	2.26	0.53
1:A:77:ILE:HG22	2:E:51:GLU:HG3	1.90	0.53
1:A:168:GLU:OE1	1:A:192:ARG:NH1	2.41	0.53
1:B:160:ILE:HG23	1:B:199:PHE:CE1	2.39	0.53
1:D:140:LEU:O	1:D:146:ILE:HG12	2.08	0.53
2:E:89:PHE:CE2	2:E:113:ARG:HG2	2.43	0.53
1:A:50:TYR:HD1	1:A:82:THR:HG22	1.73	0.53
1:A:115:ASN:O	1:A:116:LEU:HB2	2.08	0.53
1:C:122:LEU:HD12	1:C:196:MET:HE1	1.90	0.53
2:F:10:ARG:HA	2:F:113:ARG:H	1.73	0.53
1:A:76:TYR:HD1	1:A:77:ILE:HG12	1.73	0.53
1:D:6:ILE:HG13	1:D:10:LYS:CG	2.39	0.53
1:D:98:VAL:HG22	1:D:99:ASN:N	2.22	0.53
2:E:120:LEU:HD21	2:E:220:SER:OG	2.08	0.53
2:F:194:SER:O	2:F:195:ARG:CB	2.57	0.53
1:B:146:ILE:HG13	1:B:147:TYR:N	2.23	0.53
2:E:84:PRO:O	2:E:85:GLU:C	2.52	0.53
1:A:114:GLN:CD	1:A:115:ASN:N	2.67	0.53
1:D:4:LYS:O	1:D:5:ASP:O	2.27	0.53
1:D:69:VAL:CG2	1:D:90:ILE:HG23	2.27	0.53
2:E:27(A):PHE:C	2:E:27(A):PHE:CD2	2.85	0.53
2:E:60:VAL:O	2:E:61:GLU:CG	2.56	0.53
1:A:26:ASP:O	1:A:43:LYS:NZ	2.35	0.53
1:A:31:PHE:CD1	1:A:32:SER:N	2.77	0.53
1:B:196:MET:C	1:B:198:ASN:H	2.16	0.53
1:C:7:SER:C	1:C:9:VAL:N	2.60	0.53
2:E:9:SER:O	2:E:10:ARG:HB3	2.09	0.53
1:A:9:VAL:O	1:A:11:SER:N	2.42	0.53
1:D:42:GLN:O	1:D:43:LYS:CB	2.56	0.53
1:D:72:PHE:C	1:D:72:PHE:HD1	2.17	0.53
2:E:174:THR:HG22	2:E:194:SER:OG	2.08	0.53
1:B:19:ILE:HG12	1:B:20:THR:H	1.74	0.52
1:B:77:ILE:C	2:F:52:GLY:HA3	2.33	0.52
1:C:102:LEU:HD11	1:C:122:LEU:CG	2.38	0.52
1:D:45:ARG:CG	1:D:45:ARG:NH1	2.71	0.52
2:E:138:SER:O	2:E:139:HIS:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD22	1:B:199:PHE:CE2	2.43	0.52
2:F:129:VAL:O	2:F:130:PHE:CD1	2.62	0.52
1:B:4:LYS:NZ	1:B:4:LYS:CB	2.73	0.52
1:C:45:ARG:HG3	1:C:45:ARG:NH1	2.23	0.52
2:E:153:TYR:CB	2:E:154:PRO:HD3	2.33	0.52
2:E:122:ASN:O	2:E:123:PHE:CB	2.56	0.52
2:E:172:VAL:HG12	2:E:196:LEU:CD1	2.38	0.52
2:E:233:VAL:O	2:E:235:GLN:N	2.42	0.52
1:A:10:LYS:HZ1	1:A:151:SER:HB3	1.73	0.52
1:A:43:LYS:HE3	1:A:44:TYR:CE2	2.45	0.52
1:D:55:MET:HE3	1:D:59:ALA:C	2.34	0.52
1:B:63:PHE:CD2	1:B:90:ILE:HD11	2.45	0.52
1:B:106:LEU:HD23	1:B:106:LEU:C	2.35	0.52
1:D:39:ILE:HD13	1:D:69:VAL:CG1	2.40	0.52
1:B:72:PHE:C	1:B:72:PHE:HD1	2.17	0.52
1:B:131:GLU:CG	1:B:135:LYS:HE3	2.40	0.52
1:C:87:TYR:CD2	1:C:186:ALA:HA	2.44	0.52
1:C:154:VAL:HG22	1:C:154:VAL:O	2.10	0.52
1:D:129:PHE:HA	1:D:132:ILE:CG2	2.39	0.52
1:D:146:ILE:O	1:D:147:TYR:C	2.53	0.52
2:E:14:LYS:HG3	2:E:15:SER:H	1.74	0.52
1:A:30:ASN:C	1:A:30:ASN:ND2	2.66	0.52
1:B:30:ASN:N	1:B:38:ASN:O	2.42	0.52
2:E:62:LYS:HA	2:E:62:LYS:CE	2.25	0.52
1:A:109:SER:OG	1:A:207:GLU:HA	2.10	0.52
1:B:164:ASP:O	1:B:165:GLY:C	2.53	0.52
2:F:17:THR:N	2:F:81:SER:OG	2.43	0.52
2:F:234:THR:O	2:F:235:GLN:HB2	2.09	0.52
1:A:9:VAL:C	1:A:11:SER:H	2.17	0.52
1:A:184:ILE:C	1:A:186:ALA:N	2.66	0.52
1:B:195:ASN:ND2	1:B:197:LYS:H	2.08	0.52
2:E:83:HIS:C	2:E:116:VAL:HG21	2.34	0.52
1:B:10:LYS:HE2	1:B:146:ILE:O	2.10	0.51
1:B:75:PHE:CD1	1:B:75:PHE:C	2.88	0.51
1:B:85:TYR:O	1:B:86:ILE:HG23	2.10	0.51
1:C:157:ARG:HH21	1:C:205:TYR:C	2.18	0.51
1:D:39:ILE:HD11	1:D:90:ILE:HD12	1.92	0.51
1:D:156:GLY:O	1:D:157:ARG:NH1	2.44	0.51
2:E:80:THR:O	2:E:81:SER:O	2.28	0.51
2:F:87:SER:O	2:F:88:SER:OG	2.28	0.51
1:C:7:SER:O	1:C:8:ASN:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD23	1:C:14:LEU:C	2.34	0.51
2:E:30:THR:O	2:E:30:THR:OG1	2.19	0.51
2:E:168:VAL:HG22	2:E:169:HIS:N	2.25	0.51
1:A:79:ASN:C	1:A:81:HIS:N	2.56	0.51
1:C:202:PHE:CD1	1:C:202:PHE:C	2.87	0.51
1:D:77:ILE:CG1	1:D:78:LEU:N	2.74	0.51
2:F:48:THR:OG1	2:F:49:SER:N	2.44	0.51
2:F:65:PHE:HD2	2:F:79:VAL:HG12	1.76	0.51
1:A:94:GLN:NE2	1:A:125:ASP:N	2.48	0.51
1:D:13:LEU:HD22	1:D:147:TYR:CZ	2.45	0.51
2:F:14:LYS:O	2:F:17:THR:HB	2.11	0.51
2:F:205:ASN:CG	2:F:206:PRO:HD2	2.35	0.51
2:E:97:GLY:O	2:E:98:SER:HB2	2.11	0.51
2:E:136:GLU:OE1	2:E:144:THR:HG22	2.10	0.51
1:A:160:ILE:HG23	1:A:199:PHE:CE1	2.46	0.51
2:F:19:VAL:HG12	2:F:21:ILE:HG13	1.93	0.51
1:A:181:ARG:NH1	2:E:52(A):SER:OG	2.43	0.51
1:B:197:LYS:HA	1:D:163:LYS:HE3	1.92	0.51
1:C:152:PRO:O	1:C:208:LYS:HG2	2.11	0.51
1:D:29:VAL:HG11	1:D:64:LYS:C	2.36	0.51
2:E:153:TYR:CB	2:E:154:PRO:CD	2.89	0.51
2:E:186:ASN:O	2:E:187:ASP:HB3	2.10	0.51
1:B:60:SER:C	1:B:62:LYS:H	2.18	0.51
1:B:176:PRO:HD2	1:B:184:ILE:HG13	1.93	0.51
1:C:6:ILE:HD13	1:C:7:SER:N	2.26	0.51
2:E:21:ILE:HD12	2:E:77:LEU:CD1	2.41	0.51
1:B:106:LEU:HD21	1:B:108:ILE:HG13	1.93	0.50
1:C:157:ARG:NE	1:C:205:TYR:HB2	2.26	0.50
2:E:14:LYS:NZ	2:E:223:ASP:OD2	2.45	0.50
2:E:186:ASN:O	2:E:188:SER:N	2.43	0.50
1:D:102:LEU:HD12	1:D:120:ILE:CG2	2.28	0.50
1:A:77:ILE:C	1:A:78:LEU:CD1	2.81	0.50
2:E:233:VAL:HG23	2:E:234:THR:N	2.25	0.50
2:F:11:VAL:HG22	2:F:12:ILE:N	2.26	0.50
2:F:74:LEU:CG	2:F:75:SER:N	2.74	0.50
1:A:16:ALA:HA	1:A:181:ARG:HE	1.74	0.50
1:A:55:MET:HE2	1:A:191:ASN:HB2	1.94	0.50
1:C:19:ILE:HD11	1:C:75:PHE:CE2	2.46	0.50
1:A:178:GLU:HB3	1:A:183:ASP:OD2	2.11	0.50
1:D:108:ILE:HG12	1:D:206:LEU:HB2	1.93	0.50
2:E:180:LYS:HE3	2:E:188:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:THR:HG22	2:F:74:LEU:N	2.26	0.50
1:A:181:ARG:N	2:E:53:LYS:O	2.41	0.50
1:C:97:LYS:C	1:C:98:VAL:HG13	2.37	0.50
1:D:39:ILE:CD1	1:D:69:VAL:HG11	2.42	0.50
2:E:135:ALA:O	2:E:138:SER:O	2.30	0.50
2:E:166:LYS:HB3	2:E:167:GLU:OE1	2.12	0.50
2:F:22:GLU:O	2:F:24:ARG:HG3	2.10	0.50
1:A:78:LEU:HD22	2:E:52:GLY:CA	2.39	0.50
1:A:185:PHE:N	1:A:185:PHE:CD1	2.79	0.50
1:B:148:ASP:O	1:B:149:ALA:C	2.55	0.50
2:E:37:GLN:HG3	2:E:42:SER:HA	1.93	0.50
2:E:63:ASP:OD1	2:E:64:LYS:HD2	2.10	0.50
2:F:17:THR:H	2:F:81:SER:HB2	1.76	0.50
1:B:133:ASP:OD2	1:B:188:TYR:OH	2.18	0.50
1:C:144:TYR:O	1:C:145:LYS:C	2.54	0.50
2:E:3:VAL:HG22	2:E:4:VAL:N	2.27	0.50
1:A:101:LYS:HD3	1:A:118:ASN:OD1	2.12	0.50
1:B:69:VAL:HG22	1:B:70:ASP:N	2.27	0.50
2:E:65:PHE:HE1	2:E:79:VAL:HG23	1.77	0.50
1:B:94:GLN:HG3	1:B:96:ASN:O	2.12	0.49
1:B:106:LEU:HD12	1:B:204:ILE:HD11	1.94	0.49
1:C:17:TYR:O	1:C:19:ILE:HG22	2.12	0.49
1:C:77:ILE:HG12	1:C:78:LEU:H	1.76	0.49
1:D:42:GLN:O	1:D:43:LYS:CG	2.59	0.49
2:E:98:SER:O	2:E:100:SER:N	2.45	0.49
2:E:182:GLN:O	2:E:185:LEU:CD2	2.60	0.49
2:E:226:THR:CG2	2:E:227:GLN:N	2.60	0.49
1:C:39:ILE:HG22	1:C:40:ASP:N	2.27	0.49
2:E:10:ARG:O	2:E:11:VAL:HG23	2.13	0.49
2:E:125:PRO:HB3	2:E:152:PHE:CB	2.38	0.49
1:B:64:LYS:HD3	1:B:65:ARG:N	2.27	0.49
1:C:106:LEU:CD1	1:C:144:TYR:CZ	2.95	0.49
1:D:10:LYS:HB3	1:D:147:TYR:HA	1.94	0.49
2:E:8:PRO:CG	2:E:21:ILE:HA	2.43	0.49
2:E:159:LEU:HD22	2:E:174:THR:CG2	2.40	0.49
2:F:30:THR:CG2	2:F:31:THR:H	2.13	0.49
1:A:114:GLN:NE2	1:A:115:ASN:N	2.61	0.49
1:B:64:LYS:HD3	1:B:65:ARG:O	2.11	0.49
1:C:85:TYR:N	1:C:85:TYR:CD1	2.80	0.49
1:C:97:LYS:O	1:C:98:VAL:CG1	2.61	0.49
1:C:177:ASN:HB2	1:C:183:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ILE:HG23	1:D:133:ASP:N	2.27	0.49
2:F:13:ALA:O	2:F:115:THR:O	2.30	0.49
1:A:23:ASP:HA	1:A:71:VAL:O	2.13	0.49
1:A:69:VAL:HG22	1:A:70:ASP:N	2.26	0.49
1:C:6:ILE:CG2	1:C:7:SER:N	2.69	0.49
2:E:113:ARG:NH2	2:E:155:ASP:OD2	2.46	0.49
2:E:230:ALA:O	2:E:231:LYS:C	2.56	0.49
1:B:56:SER:O	1:B:59:ALA:HB3	2.11	0.49
1:B:69:VAL:CG2	1:B:90:ILE:CD1	2.89	0.49
1:C:141:MET:O	1:C:145:LYS:HD3	2.12	0.49
1:D:100:HIS:N	1:D:122:LEU:O	2.22	0.49
1:A:79:ASN:OD1	2:E:97:GLY:N	2.45	0.49
1:B:89:GLY:HA3	1:B:130:GLN:NE2	2.27	0.49
1:D:84:GLU:C	1:D:85:TYR:HD1	2.21	0.49
2:E:8:PRO:HG3	2:E:22:GLU:H	1.77	0.49
2:E:72:LEU:HD23	2:E:72:LEU:H	1.77	0.49
2:E:107:TYR:O	2:E:108:PHE:HD1	1.94	0.49
2:F:41:GLN:O	2:F:42:SER:HB3	2.12	0.49
1:A:57:TYR:C	1:A:59:ALA:H	2.20	0.49
1:A:137:ARG:NH2	1:A:187:LYS:NZ	2.61	0.49
1:B:64:LYS:HE2	1:B:65:ARG:H	1.77	0.49
1:B:164:ASP:OD1	1:B:198:ASN:OD1	2.31	0.49
1:C:22:TYR:O	1:C:72:PHE:HA	2.13	0.49
1:C:65:ARG:HG3	1:C:66:ASP:N	2.27	0.49
1:C:170:ILE:HG22	1:C:170:ILE:O	2.13	0.49
1:D:70:ASP:OD1	1:D:93:ALA:HA	2.12	0.49
2:E:219:LEU:HD21	2:E:232:PRO:O	2.13	0.49
1:A:4:LYS:NZ	1:A:154:VAL:HG22	2.28	0.49
2:E:240:GLU:OE2	2:E:242:TRP:HZ3	1.95	0.49
1:A:94:GLN:NE2	1:A:124:LYS:HA	2.18	0.49
1:D:156:GLY:C	1:D:157:ARG:HH11	2.21	0.49
2:F:33:PHE:CD1	2:F:33:PHE:N	2.79	0.49
1:B:14:LEU:HD23	1:B:14:LEU:C	2.35	0.48
1:C:76:TYR:CE1	1:C:77:ILE:HG22	2.48	0.48
1:D:77:ILE:CG1	1:D:78:LEU:H	2.25	0.48
2:E:84:PRO:HA	2:E:116:VAL:HG23	1.94	0.48
2:E:172:VAL:HA	2:E:195:ARG:O	2.13	0.48
1:B:195:ASN:ND2	1:B:197:LYS:N	2.61	0.48
1:A:100:HIS:O	1:A:121:ILE:HG23	2.13	0.48
1:A:102:LEU:CD2	1:A:196:MET:HE1	2.44	0.48
1:C:202:PHE:CD1	1:C:202:PHE:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:GLY:O	2:E:52(A):SER:CB	2.57	0.48
2:F:234:THR:O	2:F:235:GLN:HG2	2.12	0.48
1:A:17:TYR:O	1:A:19:ILE:HG22	2.13	0.48
1:A:102:LEU:HD12	1:A:120:ILE:CG2	2.40	0.48
1:C:75:PHE:CD1	1:C:75:PHE:C	2.92	0.48
2:F:12:ILE:HD12	2:F:234:THR:H	1.78	0.48
1:A:102:LEU:HD22	1:A:199:PHE:CE2	2.48	0.48
1:B:56:SER:O	1:B:59:ALA:N	2.46	0.48
1:A:202:PHE:CD1	1:A:202:PHE:O	2.66	0.48
1:B:19:ILE:HD12	1:B:181:ARG:CZ	2.43	0.48
1:C:9:VAL:C	1:C:11:SER:N	2.68	0.48
2:E:8:PRO:HG2	2:E:21:ILE:HA	1.95	0.48
1:A:6:ILE:HG23	1:A:7:SER:N	2.27	0.48
1:B:37:LEU:HB2	1:B:55:MET:CE	2.44	0.48
1:B:76:TYR:HA	1:B:181:ARG:CB	2.31	0.48
2:E:68:ASN:N	2:E:68:ASN:ND2	2.61	0.48
1:C:154:VAL:HG13	1:C:155:SER:OG	2.13	0.48
1:D:27:CYS:O	1:D:69:VAL:N	2.44	0.48
2:E:52(A):SER:C	2:E:54:ALA:N	2.67	0.48
2:F:12:ILE:CD1	2:F:234:THR:H	2.27	0.48
1:A:39:ILE:CD1	1:A:90:ILE:HD13	2.44	0.48
1:B:19:ILE:HD11	1:B:75:PHE:CE2	2.49	0.47
1:B:29:VAL:HG11	1:B:37:LEU:HD11	1.95	0.47
2:E:83:HIS:O	2:E:116:VAL:HG21	2.14	0.47
1:A:50:TYR:CD1	1:A:82:THR:HG22	2.49	0.47
1:B:87:TYR:CD2	1:B:185:PHE:C	2.92	0.47
1:B:89:GLY:CA	1:B:130:GLN:NE2	2.77	0.47
1:B:144:TYR:O	1:B:145:LYS:C	2.57	0.47
1:B:157:ARG:NE	1:B:159:GLU:OE2	2.47	0.47
2:E:33:PHE:HD1	2:E:93:SER:OG	1.96	0.47
2:E:36:ARG:HB2	2:E:46:MET:SD	2.54	0.47
2:F:233:VAL:O	2:F:234:THR:OG1	2.30	0.47
1:B:186:ALA:C	1:B:188:TYR:H	2.22	0.47
1:B:196:MET:C	1:B:198:ASN:N	2.71	0.47
1:D:94:GLN:HE22	1:D:125:ASP:H	1.62	0.47
2:E:31:THR:HG23	2:E:49:SER:O	2.14	0.47
2:F:72:LEU:HD23	2:F:72:LEU:H	1.79	0.47
1:A:79:ASN:O	1:A:79:ASN:CG	2.57	0.47
1:D:130:GLN:HA	1:D:188:TYR:CE1	2.49	0.47
2:E:40:LYS:O	2:E:41:GLN:CB	2.62	0.47
2:F:86:ASP:OD2	2:F:116:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:HB2	1:B:38:ASN:OD1	2.15	0.47
1:B:163:LYS:HA	1:B:163:LYS:HD3	1.71	0.47
1:B:168:GLU:OE2	1:B:192:ARG:NH1	2.47	0.47
1:C:87:TYR:CE2	1:C:186:ALA:HA	2.49	0.47
1:C:180:THR:H	1:C:183:ASP:HB2	1.79	0.47
2:F:12:ILE:HD12	2:F:233:VAL:CA	2.44	0.47
2:F:74:LEU:HG	2:F:75:SER:H	1.78	0.47
2:F:116:VAL:HG12	2:F:116:VAL:O	2.13	0.47
1:B:131:GLU:HG3	1:B:135:LYS:HE3	1.95	0.47
1:C:177:ASN:O	1:C:178:GLU:C	2.58	0.47
2:E:110:PRO:O	2:E:111:GLY:O	2.33	0.47
2:E:226:THR:CG2	2:E:227:GLN:HG3	2.44	0.47
2:F:72:LEU:HD23	2:F:72:LEU:N	2.29	0.47
1:B:7:SER:O	1:B:9:VAL:N	2.47	0.47
1:B:119:LYS:O	1:B:120:ILE:HG13	2.15	0.47
1:B:138:LYS:O	1:B:139:TYR:C	2.58	0.47
1:B:181:ARG:NH1	2:F:52(A):SER:OG	2.48	0.47
1:B:195:ASN:HD22	1:B:197:LYS:N	2.13	0.47
1:C:17:TYR:C	1:C:19:ILE:N	2.71	0.47
1:D:167:HIS:ND1	1:D:167:HIS:C	2.72	0.47
2:E:14:LYS:HE2	2:E:222:ASN:N	2.30	0.47
2:E:118:GLU:HG3	2:E:119:ASP:H	1.80	0.47
2:E:229:ARG:C	2:E:231:LYS:H	2.23	0.47
1:A:190:ASP:CG	1:A:192:ARG:HB2	2.40	0.47
2:E:15:SER:HB3	2:E:83:HIS:CE1	2.50	0.47
2:E:60:VAL:O	2:E:61:GLU:HG2	2.15	0.47
2:E:172:VAL:HG12	2:E:196:LEU:HD13	1.96	0.47
1:B:75:PHE:CE1	1:B:181:ARG:NH1	2.83	0.47
1:C:72:PHE:CD1	1:C:72:PHE:C	2.91	0.47
1:D:155:SER:HA	1:D:173:PHE:CD1	2.50	0.47
2:E:180:LYS:NZ	2:E:184:ALA:HA	2.30	0.47
2:F:194:SER:OG	2:F:195:ARG:N	2.45	0.47
1:A:9:VAL:O	1:A:10:LYS:C	2.57	0.47
1:C:22:TYR:CE1	1:C:84:GLU:OE2	2.68	0.47
1:C:24:TYR:CE2	1:C:51:ILE:HD11	2.47	0.47
1:D:76:TYR:HB2	1:D:182:SER:HB2	1.96	0.47
2:E:56:TYR:CD2	2:E:57:GLU:N	2.76	0.47
2:E:62:LYS:HE2	2:E:62:LYS:CA	2.29	0.47
2:E:125:PRO:HB3	2:E:152:PHE:CD1	2.49	0.47
2:E:180:LYS:HZ3	2:E:184:ALA:HA	1.79	0.47
2:F:12:ILE:CD1	2:F:234:THR:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:ASN:OD1	2:F:206:PRO:HD2	2.14	0.47
1:A:10:LYS:O	1:A:14:LEU:HB2	2.15	0.46
1:B:6:ILE:HG13	1:B:7:SER:H	1.78	0.46
2:E:125:PRO:CB	2:E:152:PHE:HB3	2.40	0.46
2:E:142:LYS:CD	2:E:197:ARG:HE	2.28	0.46
2:F:88:SER:O	2:F:89:PHE:C	2.58	0.46
1:B:141:MET:O	1:B:142:ASP:C	2.58	0.46
1:D:69:VAL:HG22	1:D:70:ASP:N	2.30	0.46
1:A:39:ILE:N	1:A:39:ILE:HD12	2.30	0.46
1:A:63:PHE:HB3	1:A:67:ASP:OD2	2.14	0.46
1:D:41:THR:CG2	1:D:51:ILE:HG12	2.45	0.46
1:D:129:PHE:C	1:D:132:ILE:HG22	2.40	0.46
1:D:195:ASN:ND2	1:D:197:LYS:HB3	2.29	0.46
2:E:236:ILE:O	2:E:236:ILE:HG23	2.14	0.46
2:F:62:LYS:HD2	2:F:65:PHE:CE1	2.51	0.46
2:F:86:ASP:CG	2:F:116:VAL:HG23	2.41	0.46
2:F:129:VAL:CG2	2:F:239:ALA:HB1	2.46	0.46
1:A:130:GLN:HG3	1:A:188:TYR:CE2	2.51	0.46
1:B:72:PHE:CZ	1:B:131:GLU:HG3	2.50	0.46
1:B:74:LEU:CB	1:B:185:PHE:CE2	2.99	0.46
1:B:119:LYS:C	1:B:120:ILE:HG13	2.40	0.46
1:B:200:SER:O	1:B:201:HIS:CB	2.61	0.46
1:D:22:TYR:O	1:D:72:PHE:HA	2.15	0.46
2:E:26:LEU:HD23	2:E:26:LEU:C	2.39	0.46
1:C:34:THR:CG2	1:C:34:THR:O	2.63	0.46
2:E:219:LEU:CD1	2:E:220:SER:HB2	2.45	0.46
1:A:201:HIS:HB3	1:C:103:LEU:CD1	2.46	0.46
1:D:85:TYR:N	1:D:85:TYR:CD1	2.83	0.46
1:D:100:HIS:O	1:D:122:LEU:N	2.42	0.46
2:E:95:LEU:HD22	2:E:96:ALA:H	1.81	0.46
2:E:214:VAL:HB	2:E:237:VAL:CG2	2.36	0.46
1:A:69:VAL:HG23	1:A:91:THR:O	2.15	0.46
1:A:191:ASN:C	1:A:191:ASN:ND2	2.74	0.46
1:B:29:VAL:HG22	1:B:39:ILE:HG12	1.98	0.46
1:D:104:GLY:H	1:D:117:ASN:HD22	1.64	0.46
2:E:227:GLN:HG2	2:E:231:LYS:CD	2.39	0.46
2:F:77:LEU:HD23	2:F:77:LEU:C	2.40	0.46
1:A:28:ARG:H	1:A:28:ARG:CD	2.14	0.46
1:C:115:ASN:O	1:C:116:LEU:HD23	2.16	0.46
2:E:137:ILE:O	2:E:141:GLN:NE2	2.48	0.46
1:A:53:SER:HB2	1:A:90:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:O	1:A:56:SER:C	2.59	0.46
1:A:138:LYS:NZ	1:A:142:ASP:OD2	2.49	0.46
1:B:21:PRO:HB3	1:B:74:LEU:HD23	1.98	0.46
2:E:82:ALA:HB1	2:E:116:VAL:HG12	1.98	0.46
2:E:136:GLU:OE2	2:E:144:THR:HG23	2.16	0.46
2:F:22:GLU:HB2	2:F:74:LEU:CD1	2.46	0.46
1:A:63:PHE:CE1	1:A:92:PRO:HG3	2.51	0.45
2:E:20:LYS:H	2:E:20:LYS:CD	2.26	0.45
2:E:120:LEU:HD21	2:E:220:SER:CA	2.46	0.45
2:E:206:PRO:O	2:E:208:ASN:N	2.48	0.45
1:A:91:THR:O	1:A:92:PRO:C	2.59	0.45
2:F:6:GLN:NE2	2:F:90:TYR:O	2.34	0.45
1:A:139:TYR:O	1:A:140:LEU:CG	2.64	0.45
1:D:120:ILE:HD11	1:D:139:TYR:HB2	1.97	0.45
2:E:14:LYS:HG3	2:E:15:SER:N	2.32	0.45
2:E:205:ASN:CG	2:E:205:ASN:O	2.59	0.45
2:F:37:GLN:O	2:F:88:SER:OG	2.35	0.45
1:B:24:TYR:CD2	1:B:41:THR:HG21	2.50	0.45
1:C:55:MET:CE	1:C:60:SER:HA	2.47	0.45
1:D:29:VAL:CG1	1:D:64:LYS:C	2.89	0.45
2:E:59:GLY:O	2:E:60:VAL:HB	2.16	0.45
2:E:120:LEU:HD21	2:E:220:SER:CB	2.46	0.45
1:A:3:LYS:NZ	1:D:61:GLN:CB	2.80	0.45
1:B:140:LEU:HD21	1:B:204:ILE:HD12	1.98	0.45
1:C:108:ILE:H	1:C:112:SER:HA	1.82	0.45
1:D:108:ILE:O	1:D:111:GLU:O	2.34	0.45
2:F:20:LYS:O	2:F:21:ILE:HG13	2.16	0.45
1:C:75:PHE:CZ	1:C:181:ARG:NH1	2.85	0.45
2:E:225:TRP:O	2:E:226:THR:O	2.35	0.45
2:F:9:SER:O	2:F:112:THR:HA	2.16	0.45
1:A:28:ARG:HG3	1:A:28:ARG:NH1	2.29	0.45
1:A:75:PHE:C	1:A:75:PHE:HD1	2.22	0.45
1:A:79:ASN:CB	2:E:30:THR:HG21	2.44	0.45
1:B:75:PHE:HA	1:B:86:ILE:HG22	1.98	0.45
1:B:80:SER:O	1:B:81:HIS:HB2	2.16	0.45
1:D:178:GLU:O	1:D:180:THR:HG23	2.16	0.45
1:B:31:PHE:CD1	1:B:31:PHE:C	2.94	0.45
1:B:75:PHE:O	1:B:185:PHE:CE2	2.69	0.45
1:C:90:ILE:H	1:C:191:ASN:HD21	1.65	0.45
1:B:102:LEU:HD11	1:B:122:LEU:HD21	1.99	0.45
2:E:19:VAL:H	2:E:79:VAL:HG12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG21	1:A:100:HIS:CE1	2.52	0.45
1:D:60:SER:O	1:D:61:GLN:C	2.60	0.45
2:E:14:LYS:HG2	2:E:223:ASP:HB2	1.99	0.45
2:E:125:PRO:HB3	2:E:152:PHE:CG	2.52	0.45
1:B:87:TYR:CD2	1:B:185:PHE:O	2.70	0.44
1:C:192:ARG:HE	1:C:192:ARG:HB3	1.58	0.44
2:E:68:ASN:HD21	2:E:76:THR:HG1	1.62	0.44
2:F:42:SER:O	2:F:44:MET:N	2.49	0.44
1:B:8:ASN:HD22	1:B:8:ASN:H	1.62	0.44
1:C:28:ARG:HA	1:C:67:ASP:O	2.17	0.44
1:C:64:LYS:O	1:C:65:ARG:C	2.59	0.44
1:C:106:LEU:C	1:C:106:LEU:CD2	2.90	0.44
1:C:140:LEU:HB3	1:C:146:ILE:HD12	2.00	0.44
1:D:43:LYS:HG3	1:D:43:LYS:O	2.16	0.44
2:F:12:ILE:HD12	2:F:234:THR:N	2.33	0.44
1:C:9:VAL:O	1:C:13:LEU:HD12	2.16	0.44
1:C:162:THR:HG21	1:C:164:ASP:OD2	2.18	0.44
1:D:64:LYS:HZ3	1:D:65:ARG:CG	2.31	0.44
1:D:144:TYR:O	1:D:145:LYS:C	2.60	0.44
2:F:5:SER:OG	2:F:6:GLN:N	2.51	0.44
1:B:104:GLY:H	1:B:117:ASN:ND2	2.16	0.44
1:B:157:ARG:CG	1:B:157:ARG:NH1	2.78	0.44
2:E:16:GLY:H	2:E:82:ALA:HB3	1.80	0.44
2:F:129:VAL:C	2:F:130:PHE:N	2.76	0.44
2:F:192:LEU:N	2:F:192:LEU:CD1	2.78	0.44
1:A:46:GLY:O	1:A:49:TYR:HD1	2.00	0.44
1:A:85:TYR:CD1	1:A:85:TYR:N	2.85	0.44
1:A:115:ASN:HB3	1:C:115:ASN:HD21	1.82	0.44
1:B:144:TYR:O	1:B:145:LYS:O	2.36	0.44
1:C:76:TYR:HB2	1:C:182:SER:HA	1.99	0.44
1:D:4:LYS:O	1:D:5:ASP:C	2.60	0.44
1:D:7:SER:O	1:D:8:ASN:HB2	2.17	0.44
2:E:110:PRO:C	2:E:111:GLY:O	2.58	0.44
1:B:50:TYR:CD1	1:B:82:THR:O	2.71	0.44
1:B:102:LEU:HD11	1:B:122:LEU:HD23	1.96	0.44
1:C:91:THR:HB	1:C:92:PRO:CD	2.46	0.44
2:E:92:CYS:O	2:E:93:SER:HB3	2.17	0.44
2:E:162:TRP:CB	2:E:211:ARG:HG2	2.48	0.44
1:D:174:ASP:CG	1:D:175:SER:H	2.25	0.44
1:A:31:PHE:CE1	1:A:33:THR:HG23	2.31	0.44
1:B:19:ILE:CG1	1:B:20:THR:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:O	1:B:132:ILE:C	2.59	0.44
2:E:32:MET:HB3	2:E:32:MET:HE2	1.84	0.44
2:F:36:ARG:NH1	2:F:65:PHE:CE1	2.86	0.44
1:A:168:GLU:CD	1:A:192:ARG:HH12	2.25	0.44
1:D:5:ASP:C	1:D:7:SER:N	2.74	0.44
2:E:19:VAL:O	2:E:78:THR:HA	2.18	0.44
2:E:63:ASP:C	2:E:65:PHE:N	2.75	0.44
2:F:209:HIS:HB3	2:F:240:GLU:HG3	2.00	0.44
1:B:119:LYS:O	1:B:120:ILE:CG1	2.66	0.43
1:D:75:PHE:CE1	1:D:181:ARG:NH1	2.86	0.43
2:E:136:GLU:HG2	2:E:140:THR:HG21	2.00	0.43
2:E:173:SER:O	2:E:194:SER:HA	2.18	0.43
1:C:140:LEU:HD11	1:C:204:ILE:HG21	2.00	0.43
1:D:184:ILE:O	1:D:184:ILE:HD12	2.18	0.43
2:E:201:THR:HA	2:E:204:GLN:CG	2.47	0.43
1:A:55:MET:HG3	1:A:60:SER:CB	2.48	0.43
1:A:133:ASP:CG	1:A:137:ARG:HE	2.26	0.43
1:B:139:TYR:C	1:B:139:TYR:CD2	2.96	0.43
1:C:127:VAL:CG1	1:C:132:ILE:HG13	2.49	0.43
2:E:50:ALA:O	2:E:51:GLU:C	2.61	0.43
2:F:129:VAL:C	2:F:130:PHE:CA	2.86	0.43
1:A:29:VAL:O	1:A:65:ARG:C	2.62	0.43
1:A:124:LYS:HB3	1:A:126:ILE:O	2.19	0.43
1:B:14:LEU:HD23	1:B:15:TYR:H	1.75	0.43
1:B:77:ILE:HA	2:F:52(A):SER:H	1.83	0.43
1:D:91:THR:O	1:D:92:PRO:C	2.61	0.43
1:D:127:VAL:HG12	1:D:128:THR:O	2.18	0.43
2:E:42:SER:O	2:E:43:LEU:HB2	2.18	0.43
1:B:24:TYR:OH	1:B:84:GLU:OE2	2.33	0.43
1:C:110:GLY:O	1:C:111:GLU:HB3	2.18	0.43
2:E:37:GLN:O	2:E:37:GLN:HG2	2.19	0.43
2:F:86:ASP:O	2:F:114:LEU:C	2.62	0.43
1:A:114:GLN:NE2	1:A:115:ASN:HB2	2.34	0.43
1:A:154:VAL:O	1:A:155:SER:OG	2.32	0.43
1:B:16:ALA:C	1:B:18:THR:H	2.25	0.43
1:B:146:ILE:HD11	1:B:147:TYR:CZ	2.54	0.43
1:C:69:VAL:HG23	1:C:91:THR:O	2.19	0.43
1:D:50:TYR:CZ	1:D:83:GLY:HA3	2.53	0.43
2:E:203:TRP:O	2:E:243:GLY:HA3	2.19	0.43
2:F:47:ALA:HB3	2:F:67:ILE:CG2	2.40	0.43
1:A:55:MET:HA	1:A:189:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:CG2	1:A:199:PHE:CE1	3.01	0.43
1:B:157:ARG:HB2	1:B:170:ILE:O	2.19	0.43
1:B:178:GLU:HB3	1:B:183:ASP:OD2	2.19	0.43
1:D:64:LYS:HG2	1:D:65:ARG:N	2.33	0.43
1:A:14:LEU:C	1:A:14:LEU:CD2	2.92	0.43
1:B:60:SER:O	1:B:62:LYS:HB2	2.18	0.43
1:C:134:PHE:O	1:C:135:LYS:C	2.59	0.43
1:D:75:PHE:CZ	1:D:181:ARG:NH1	2.87	0.43
1:D:129:PHE:CE1	1:D:192:ARG:HG2	2.54	0.43
2:E:87:SER:OG	2:E:115:THR:HA	2.18	0.43
2:E:163:VAL:HG22	2:E:210:PHE:HE1	1.84	0.43
2:F:234:THR:O	2:F:235:GLN:CG	2.67	0.43
1:A:163:LYS:HG2	1:A:198:ASN:HA	1.99	0.43
2:F:20:LYS:O	2:F:21:ILE:CG1	2.67	0.43
2:F:127:VAL:HG23	2:F:128:ALA:N	2.32	0.43
1:A:4:LYS:HE3	1:A:154:VAL:HG22	2.00	0.43
1:B:60:SER:O	1:B:61:GLN:C	2.61	0.43
1:B:69:VAL:HG23	1:B:70:ASP:N	2.34	0.43
1:B:150:THR:O	1:B:151:SER:CB	2.66	0.43
1:D:180:THR:O	1:D:184:ILE:HG22	2.19	0.43
1:A:53:SER:HB2	1:A:90:ILE:HD11	2.01	0.42
1:A:104:GLY:CA	1:A:202:PHE:O	2.67	0.42
1:A:122:LEU:HD13	1:A:127:VAL:HG21	2.00	0.42
1:B:11:SER:CA	1:B:14:LEU:HD22	2.45	0.42
1:B:106:LEU:CG	1:B:204:ILE:HD11	2.49	0.42
1:C:129:PHE:O	1:C:133:ASP:N	2.44	0.42
2:E:159:LEU:HD22	2:E:174:THR:OG1	2.19	0.42
2:F:127:VAL:HA	2:F:150:THR:O	2.19	0.42
1:A:184:ILE:O	1:A:186:ALA:N	2.52	0.42
1:B:50:TYR:O	1:B:84:GLU:HG3	2.18	0.42
1:B:106:LEU:CD2	1:B:108:ILE:HG13	2.49	0.42
1:B:116:LEU:HD11	1:B:204:ILE:CD1	2.49	0.42
1:C:33:THR:OG1	1:C:34:THR:N	2.51	0.42
1:C:127:VAL:HG11	1:C:132:ILE:HG13	2.00	0.42
1:C:177:ASN:O	1:C:179:GLY:N	2.52	0.42
1:D:28:ARG:CZ	1:D:68:HIS:CE1	3.02	0.42
1:B:74:LEU:HB2	1:B:185:PHE:CZ	2.54	0.42
1:A:91:THR:C	1:A:92:PRO:O	2.62	0.42
1:A:199:PHE:O	1:C:163:LYS:HE3	2.19	0.42
1:B:16:ALA:HB1	1:B:181:ARG:HE	1.85	0.42
1:B:126:ILE:HD12	1:B:126:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:HG3	1:B:188:TYR:CG	2.54	0.42
1:C:76:TYR:C	1:C:76:TYR:CD1	2.98	0.42
1:C:130:GLN:HA	1:C:188:TYR:CE1	2.55	0.42
2:E:82:ALA:HB1	2:E:116:VAL:CG1	2.50	0.42
2:F:148:LEU:HD23	2:F:149:ALA:H	1.84	0.42
1:A:14:LEU:HD23	1:A:14:LEU:C	2.45	0.42
1:B:8:ASN:H	1:B:8:ASN:ND2	2.17	0.42
1:B:21:PRO:HD3	1:B:134:PHE:CE2	2.55	0.42
1:B:94:GLN:NE2	1:B:125:ASP:H	2.17	0.42
1:C:29:VAL:CG1	1:C:37:LEU:HD11	2.49	0.42
1:C:138:LYS:NZ	1:C:142:ASP:OD2	2.53	0.42
1:C:160:ILE:HB	1:C:168:GLU:HB2	2.02	0.42
1:D:9:VAL:C	1:D:11:SER:N	2.74	0.42
1:D:85:TYR:HD1	1:D:85:TYR:N	2.17	0.42
1:D:168:GLU:OE1	1:D:192:ARG:NH1	2.53	0.42
2:E:118:GLU:OE2	2:E:224:GLU:HG2	2.19	0.42
1:A:181:ARG:NH2	2:E:69:HIS:O	2.36	0.42
1:B:3:LYS:HD3	1:B:177:ASN:N	2.34	0.42
2:E:27(A):PHE:CE1	2:E:94:ALA:CB	3.01	0.42
1:A:26:ASP:N	1:A:70:ASP:OD1	2.50	0.42
1:B:28:ARG:CG	1:B:66:ASP:OD1	2.63	0.42
1:B:67:ASP:O	1:B:68:HIS:C	2.60	0.42
1:B:136:ILE:O	1:B:137:ARG:C	2.62	0.42
1:B:175:SER:HA	1:B:176:PRO:HD2	1.89	0.42
1:C:61:GLN:HE21	1:C:61:GLN:HB3	1.70	0.42
1:D:102:LEU:HD11	1:D:122:LEU:CG	2.36	0.42
1:D:6:ILE:HD12	1:D:6:ILE:HA	1.90	0.42
1:D:106:LEU:HD22	1:D:108:ILE:HG13	2.01	0.42
1:D:138:LYS:O	1:D:139:TYR:C	2.63	0.42
2:E:17:THR:O	2:E:81:SER:O	2.38	0.42
2:E:21:ILE:HD12	2:E:77:LEU:HD12	2.02	0.42
2:E:32:MET:O	2:E:49:SER:N	2.43	0.42
1:A:5:ASP:O	1:A:6:ILE:C	2.63	0.42
1:A:6:ILE:CG2	1:A:7:SER:N	2.83	0.42
1:B:122:LEU:HD13	1:B:122:LEU:HA	1.80	0.42
1:D:139:TYR:CE1	1:D:143:ASN:ND2	2.88	0.42
1:D:154:VAL:HG12	1:D:207:GLU:O	2.19	0.42
2:E:168:VAL:CG2	2:E:169:HIS:N	2.83	0.42
2:E:176:PRO:O	2:E:177:GLN:HB3	2.20	0.42
1:B:69:VAL:CG2	1:B:90:ILE:HD12	2.50	0.42
1:B:186:ALA:C	1:B:188:TYR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:HG11	1:D:64:LYS:CA	2.50	0.42
1:D:55:MET:CE	1:D:60:SER:HA	2.50	0.42
1:D:132:ILE:CG2	1:D:133:ASP:N	2.83	0.42
1:D:147:TYR:HE1	1:D:172:LEU:O	2.03	0.42
2:E:79:VAL:O	2:E:80:THR:CG2	2.68	0.42
1:A:39:ILE:HD11	1:A:90:ILE:HD13	2.01	0.41
1:B:55:MET:CB	1:B:59:ALA:HB3	2.48	0.41
1:B:76:TYR:CE1	1:B:85:TYR:HD2	2.38	0.41
1:B:183:ASP:C	1:B:184:ILE:HD12	2.45	0.41
1:A:10:LYS:HZ2	1:A:151:SER:HB3	1.84	0.41
1:A:98:VAL:CG2	1:A:100:HIS:CE1	3.03	0.41
1:B:21:PRO:HD3	1:B:134:PHE:CZ	2.55	0.41
1:D:174:ASP:CG	1:D:175:SER:N	2.78	0.41
2:E:67:ILE:HA	2:E:76:THR:O	2.19	0.41
2:E:90:TYR:O	2:E:112:THR:HG22	2.21	0.41
2:E:142:LYS:CD	2:E:197:ARG:HH11	2.32	0.41
1:B:49:TYR:HA	1:B:82:THR:O	2.20	0.41
1:B:71:VAL:HG12	1:B:72:PHE:N	2.34	0.41
1:C:163:LYS:HD3	1:C:163:LYS:HA	1.89	0.41
1:D:64:LYS:NZ	1:D:65:ARG:HG2	2.35	0.41
1:D:100:HIS:CD2	1:D:196:MET:HG3	2.55	0.41
2:E:199:SER:HB2	2:E:201:THR:O	2.20	0.41
2:F:40:LYS:O	2:F:41:GLN:HB2	2.20	0.41
2:F:125:PRO:HB2	2:F:126:GLU:H	1.53	0.41
1:A:64:LYS:O	1:A:67:ASP:OD1	2.38	0.41
1:C:61:GLN:H	1:C:61:GLN:HG2	1.72	0.41
1:C:151:SER:HA	1:C:152:PRO:HD3	1.61	0.41
1:A:150:THR:O	1:A:150:THR:OG1	2.33	0.41
1:B:19:ILE:CG1	1:B:20:THR:H	2.33	0.41
1:B:28:ARG:O	1:B:40:ASP:N	2.51	0.41
1:B:74:LEU:C	1:B:86:ILE:HG22	2.45	0.41
2:E:79:VAL:CG1	2:E:80:THR:N	2.69	0.41
2:E:107:TYR:O	2:E:108:PHE:CD1	2.73	0.41
2:E:122:ASN:HB3	2:E:123:PHE:H	1.54	0.41
1:B:7:SER:O	1:B:8:ASN:C	2.64	0.41
1:B:64:LYS:HZ1	1:B:65:ARG:HB3	1.80	0.41
1:B:196:MET:O	1:B:198:ASN:N	2.54	0.41
1:C:11:SER:O	1:C:12:ASP:C	2.64	0.41
2:F:115:THR:OG1	2:F:116:VAL:N	2.49	0.41
1:A:9:VAL:HG12	1:A:10:LYS:N	2.35	0.41
1:A:72:PHE:O	1:A:89:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:CG	1:C:115:ASN:CG	2.89	0.41
1:B:16:ALA:HA	1:B:181:ARG:HH21	1.84	0.41
2:F:61:GLU:O	2:F:62:LYS:HB2	2.20	0.41
1:A:119:LYS:HE2	1:A:139:TYR:CE1	2.56	0.41
2:F:74:LEU:CG	2:F:75:SER:H	2.32	0.41
1:A:53:SER:CB	1:A:90:ILE:HD12	2.50	0.41
1:A:76:TYR:HE1	1:A:77:ILE:HD11	1.86	0.41
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.84	0.41
1:B:191:ASN:HD22	1:B:191:ASN:HA	1.54	0.41
1:C:16:ALA:HA	1:C:181:ARG:HE	1.86	0.41
1:C:47:LYS:HE2	1:C:48:ASP:OD1	2.20	0.41
1:C:64:LYS:O	1:C:65:ARG:O	2.39	0.41
1:D:55:MET:HE3	1:D:60:SER:N	2.36	0.41
1:D:98:VAL:CG2	1:D:99:ASN:N	2.84	0.41
2:E:172:VAL:HG12	2:E:196:LEU:HD12	2.02	0.41
2:F:38:PHE:HB3	2:F:39:PRO:HD2	2.01	0.41
1:B:10:LYS:HG2	1:B:147:TYR:HA	2.03	0.41
1:B:16:ALA:C	1:B:18:THR:N	2.76	0.41
1:D:116:LEU:O	1:D:117:ASN:C	2.64	0.41
2:E:68:ASN:HD22	2:E:68:ASN:H	1.66	0.41
2:F:40:LYS:HB3	2:F:40:LYS:HE2	1.72	0.41
2:F:71:SER:C	2:F:73:THR:H	2.29	0.41
2:F:72:LEU:H	2:F:72:LEU:CD2	2.34	0.41
1:A:17:TYR:O	1:A:19:ILE:N	2.54	0.40
1:A:97:LYS:NZ	1:A:123:GLU:OE1	2.54	0.40
1:A:186:ALA:O	1:A:189:LYS:HB2	2.20	0.40
1:B:94:GLN:HE22	1:B:125:ASP:H	1.68	0.40
2:E:14:LYS:O	2:E:82:ALA:HB3	2.21	0.40
1:B:3:LYS:HD3	1:B:177:ASN:H	1.86	0.40
1:B:69:VAL:HG23	1:B:70:ASP:H	1.86	0.40
1:C:97:LYS:C	1:C:98:VAL:CG1	2.94	0.40
1:D:14:LEU:O	1:D:18:THR:OG1	2.31	0.40
1:D:42:GLN:O	1:D:43:LYS:HB3	2.21	0.40
2:E:17:THR:O	2:E:82:ALA:HB2	2.20	0.40
1:A:12:ASP:OD1	1:A:12:ASP:N	2.54	0.40
1:A:115:ASN:OD1	1:C:115:ASN:CG	2.65	0.40
1:B:26:ASP:OD2	1:B:26:ASP:C	2.64	0.40
1:D:28:ARG:CZ	1:D:68:HIS:HE1	2.35	0.40
2:E:27(A):PHE:O	2:E:28:GLN:HB2	2.21	0.40
2:E:83:HIS:O	2:E:85:GLU:N	2.54	0.40
2:F:130:PHE:O	2:F:131:GLU:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:OD2	1:A:94:GLN:N	2.47	0.40
1:B:108:ILE:HG12	1:B:206:LEU:CB	2.35	0.40
1:B:141:MET:HE3	1:B:147:TYR:HD2	1.87	0.40
2:E:95:LEU:HD23	2:E:95:LEU:HA	1.93	0.40
2:E:219:LEU:HD13	2:E:219:LEU:C	2.47	0.40
2:E:235:GLN:NE2	2:E:237:VAL:CG1	2.85	0.40
2:F:27(A):PHE:CE2	2:F:28:GLN:O	2.75	0.40
1:B:56:SER:O	1:B:57:TYR:C	2.62	0.40
1:B:154:VAL:CG1	1:B:155:SER:H	2.27	0.40
2:E:140:THR:HG22	2:E:142:LYS:N	2.34	0.40
2:E:198:VAL:HG23	2:E:199:SER:N	2.35	0.40
2:E:215:GLN:HG2	2:E:217:TYR:CD2	2.56	0.40
2:E:228:ASP:O	2:E:229:ARG:HB2	2.22	0.40
2:F:37:GLN:C	2:F:88:SER:HB3	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:GLN:OE1	2:E:223:ASP:OD2[1_655]	2.18	0.02

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	197/208 (95%)	145 (74%)	33 (17%)	19 (10%)	0	2
1	B	196/208 (94%)	146 (74%)	32 (16%)	18 (9%)	0	2
1	C	206/208 (99%)	152 (74%)	37 (18%)	17 (8%)	0	3
1	D	190/208 (91%)	147 (77%)	25 (13%)	18 (10%)	0	2
2	E	245/247 (99%)	143 (58%)	42 (17%)	60 (24%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	122/247 (49%)	59 (48%)	31 (25%)	32 (26%)	0	0
All	All	1156/1326 (87%)	792 (68%)	200 (17%)	164 (14%)	0	1

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	9	VAL
1	A	65	ARG
1	A	66	ASP
1	A	80	SER
1	A	115	ASN
1	B	4	LYS
1	B	7	SER
1	B	81	HIS
1	B	177	ASN
1	C	65	ARG
1	C	79	ASN
1	C	81	HIS
1	D	5	ASP
1	D	6	ILE
1	D	31	PHE
1	D	61	GLN
1	D	79	ASN
1	D	81	HIS
1	D	111	GLU
1	D	112	SER
1	D	120	ILE
1	D	146	ILE
1	D	177	ASN
1	D	179	GLY
2	E	8	PRO
2	E	27	ASP
2	E	39	PRO
2	E	42	SER
2	E	51	GLU
2	E	52(A)	SER
2	E	60	VAL
2	E	79	VAL
2	E	81	SER
2	E	98	SER
2	E	99	GLY

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Mol	Chain	Res	Type
2	E	107	TYR
2	E	120	LEU
2	E	122	ASN
2	E	123	PHE
2	E	139	HIS
2	E	153	TYR
2	E	155	ASP
2	E	220	SER
2	E	223	ASP
2	E	224	GLU
2	E	226	THR
2	E	234	THR
2	F	9	SER
2	F	27	ASP
2	F	41	GLN
2	F	42	SER
2	F	43	LEU
2	F	75	SER
2	F	87	SER
2	F	125	PRO
2	F	131	GLU
2	F	195	ARG
2	F	207	ARG
2	F	208	ASN
2	F	235	GLN
2	F	236	ILE
2	F	237	VAL
1	A	4	LYS
1	A	64	LYS
1	A	140	LEU
1	A	145	LYS
1	A	165	GLY
1	B	8	ASN
1	B	61	GLN
1	B	66	ASP
1	B	145	LYS
1	B	165	GLY
1	B	201	HIS
1	C	109	SER
1	C	113	GLN
1	C	178	GLU
1	D	165	GLY

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Mol	Chain	Res	Type
2	E	11	VAL
2	E	28	GLN
2	E	64	LYS
2	E	80	THR
2	E	82	ALA
2	E	140	THR
2	E	154	PRO
2	E	167	GLU
2	E	197	ARG
2	E	227	GLN
2	E	229	ARG
2	F	7	HIS
2	F	37	GLN
2	F	81	SER
2	F	88	SER
2	F	110	PRO
2	F	115	THR
2	F	126	GLU
1	A	33	THR
1	A	79	ASN
1	B	77	ILE
1	C	6	ILE
1	C	47	LYS
1	C	112	SER
1	C	184	ILE
1	D	43	LYS
1	D	117	ASN
2	E	31	THR
2	E	41	GLN
2	E	43	LEU
2	E	62	LYS
2	E	101	SER
2	E	159	LEU
2	E	160	SER
2	E	185	LEU
2	E	206	PRO
2	F	8	PRO
2	F	48	THR
2	F	188	SER
1	A	77	ILE
1	A	150	THR
1	A	177	ASN

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Mol	Chain	Res	Type
1	B	5	ASP
1	B	14	LEU
1	B	151	SER
1	C	80	SER
1	D	145	LYS
2	E	29	ALA
2	E	55	THR
2	E	86	ASP
2	E	103	ASP
2	E	110	PRO
2	E	169	HIS
2	E	188	SER
2	F	30	THR
2	F	51	GLU
2	F	238	SER
1	A	185	PHE
1	B	30	ASN
1	B	35	HIS
1	C	18	THR
1	C	110	GLY
1	C	134	PHE
1	D	110	GLY
2	E	10	ARG
2	E	12	ILE
2	E	40	LYS
2	E	125	PRO
2	E	216	PHE
2	F	21	ILE
2	F	206	PRO
1	A	113	GLN
1	B	197	LYS
1	C	177	ASN
2	E	93	SER
2	E	231	LYS
2	F	239	ALA
1	B	86	ILE
1	D	77	ILE
2	E	111	GLY
1	A	152	PRO
1	C	170	ILE
2	E	233	VAL
2	F	84	PRO

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Mol	Chain	Res	Type
1	C	120	ILE
2	E	232	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	183/192 (95%)	151 (82%)	32 (18%)	2	10
1	B	175/192 (91%)	159 (91%)	16 (9%)	9	33
1	C	186/192 (97%)	166 (89%)	20 (11%)	6	26
1	D	171/192 (89%)	155 (91%)	16 (9%)	8	32
2	E	201/213 (94%)	161 (80%)	40 (20%)	1	7
2	F	108/213 (51%)	88 (82%)	20 (18%)	1	9
All	All	1024/1194 (86%)	880 (86%)	144 (14%)	3	16

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	ILE
1	A	7	SER
1	A	8	ASN
1	A	9	VAL
1	A	12	ASP
1	A	14	LEU
1	A	25	LYS
1	A	28	ARG
1	A	29	VAL
1	A	30	ASN
1	A	32	SER
1	A	47	LYS
1	A	51	ILE
1	A	54	GLU
1	A	65	ARG

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Mol	Chain	Res	Type
1	A	77	ILE
1	A	85	TYR
1	A	99	ASN
1	A	106	LEU
1	A	108	ILE
1	A	112	SER
1	A	127	VAL
1	A	128	THR
1	A	150	THR
1	A	164	ASP
1	A	166	LYS
1	A	168	GLU
1	A	191	ASN
1	A	194	ILE
1	A	195	ASN
1	A	207	GLU
1	B	4	LYS
1	B	6	ILE
1	B	14	LEU
1	B	64	LYS
1	B	69	VAL
1	B	78	LEU
1	B	79	ASN
1	B	90	ILE
1	B	98	VAL
1	B	122	LEU
1	B	128	THR
1	B	157	ARG
1	B	168	GLU
1	B	171	ASP
1	B	191	ASN
1	B	193	ILE
1	C	1	ASP
1	C	5	ASP
1	C	6	ILE
1	C	13	LEU
1	C	20	THR
1	C	34	THR
1	C	45	ARG
1	C	58	GLU
1	C	61	GLN
1	C	65	ARG

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Mol	Chain	Res	Type
1	C	71	VAL
1	C	106	LEU
1	C	127	VAL
1	C	146	ILE
1	C	155	SER
1	C	157	ARG
1	C	175	SER
1	C	195	ASN
1	C	197	LYS
1	C	200	SER
1	D	3	LYS
1	D	6	ILE
1	D	13	LEU
1	D	41	THR
1	D	45	ARG
1	D	58	GLU
1	D	63	PHE
1	D	78	LEU
1	D	85	TYR
1	D	106	LEU
1	D	111	GLU
1	D	146	ILE
1	D	157	ARG
1	D	167	HIS
1	D	177	ASN
1	D	184	ILE
2	E	4	VAL
2	E	12	ILE
2	E	14	LYS
2	E	19	VAL
2	E	39	PRO
2	E	43	LEU
2	E	44	MET
2	E	51	GLU
2	E	55	THR
2	E	58	GLN
2	E	61	GLU
2	E	67	ILE
2	E	68	ASN
2	E	77	LEU
2	E	78	THR
2	E	95	LEU

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Mol	Chain	Res	Type
2	E	102	THR
2	E	108	PHE
2	E	113	ARG
2	E	116	VAL
2	E	125	PRO
2	E	133	SER
2	E	144	THR
2	E	148	LEU
2	E	150	THR
2	E	155	ASP
2	E	167	GLU
2	E	185	LEU
2	E	195	ARG
2	E	205	ASN
2	E	207	ARG
2	E	208	ASN
2	E	211	ARG
2	E	215	GLN
2	E	224	GLU
2	E	226	THR
2	E	229	ARG
2	E	232	PRO
2	E	233	VAL
2	E	235	GLN
2	F	5	SER
2	F	7	HIS
2	F	10	ARG
2	F	20	LYS
2	F	33	PHE
2	F	35	TYR
2	F	61	GLU
2	F	67	ILE
2	F	76	THR
2	F	77	LEU
2	F	83	HIS
2	F	108	PHE
2	F	125	PRO
2	F	126	GLU
2	F	127	VAL
2	F	131	GLU
2	F	146	VAL
2	F	148	LEU

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Mol	Chain	Res	Type
2	F	187	ASP
2	F	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	81	HIS
1	A	94	GLN
1	A	105	ASN
1	A	114	GLN
1	B	8	ASN
1	B	94	GLN
1	B	100	HIS
1	B	117	ASN
1	B	130	GLN
1	B	191	ASN
1	B	195	ASN
1	B	198	ASN
1	B	201	HIS
1	C	8	ASN
1	C	30	ASN
1	C	42	GLN
1	C	61	GLN
1	C	81	HIS
1	C	94	GLN
1	C	167	HIS
1	C	191	ASN
1	D	94	GLN
1	D	117	ASN
1	D	167	HIS
1	D	177	ASN
1	D	191	ASN
1	D	195	ASN
2	E	28	GLN
2	E	37	GLN
2	E	68	ASN
2	E	122	ASN
2	E	141	GLN
2	E	156	HIS
2	E	169	HIS
2	E	208	ASN

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Mol	Chain	Res	Type
2	E	215	GLN
2	E	227	GLN
2	F	41	GLN
2	F	68	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	129:VAL	C	130:PHE	N	2.76

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	203/208 (97%)	-0.43	3 (1%)	72	49	29, 56, 87, 119	0
1	B	200/208 (96%)	-0.09	6 (3%)	52	30	49, 81, 103, 124	0
1	C	208/208 (100%)	-0.45	3 (1%)	73	51	34, 57, 84, 104	0
1	D	198/208 (95%)	-0.12	3 (1%)	72	49	50, 74, 110, 130	0
2	E	247/247 (100%)	0.13	9 (3%)	46	26	42, 80, 119, 130	0
2	F	144/247 (58%)	0.73	14 (9%)	13	7	69, 112, 137, 149	0
All	All	1200/1326 (90%)	-0.07	38 (3%)	50	29	29, 74, 123, 149	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	9	SER	4.1
1	D	110	GLY	3.7
2	F	239	ALA	3.4
2	F	208	ASN	3.4
2	F	233	VAL	3.3
1	B	34	THR	3.2
1	C	81	HIS	3.2
1	C	4	LYS	3.0
2	F	234	THR	2.9
1	A	59	ALA	2.9
2	E	96	ALA	2.8
2	E	99	GLY	2.6
2	F	39	PRO	2.5
2	E	216	PHE	2.5
1	B	171	ASP	2.4
2	E	8	PRO	2.4
2	E	201	THR	2.3
2	F	128	ALA	2.3
2	F	124	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	2.3
2	E	80	THR	2.3
2	E	155	ASP	2.3
1	D	109	SER	2.2
2	F	46	MET	2.2
1	B	177	ASN	2.2
2	F	150	THR	2.2
1	C	111	GLU	2.1
2	F	193	SER	2.1
1	A	151	SER	2.1
1	B	164	ASP	2.1
2	F	235	GLN	2.1
2	F	89	PHE	2.1
1	B	12	ASP	2.0
1	B	80	SER	2.0
1	D	30	ASN	2.0
2	F	209	HIS	2.0
2	E	38	PHE	2.0
2	E	61	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.