Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 AM UTC

PDB ID	:	3C6L / pdb_00003c6l
Title	:	Crystal structure of mouse MHC class II I-Ab/3K peptide complexed with mouse TCR 2W20
Authors	:	Dai, S.
Deposited on	:	2008-02-04
Resolution	:	3.40 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:

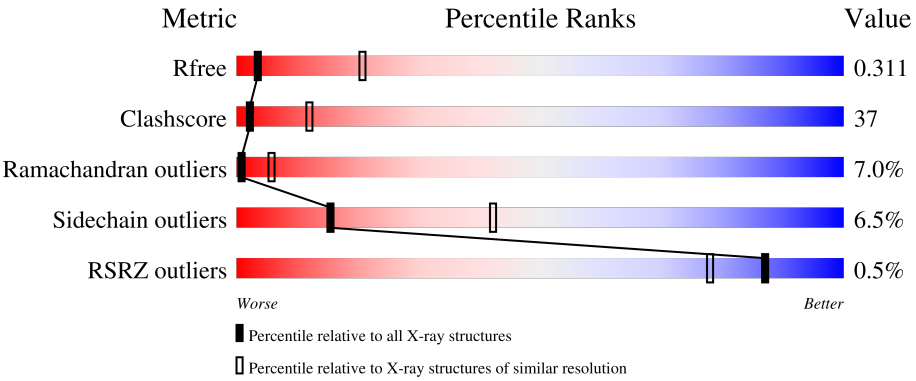
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.40 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.



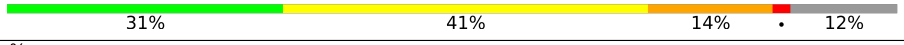
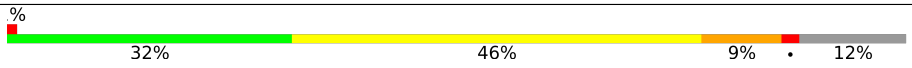
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 <=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	185	47% 41% 10%
1	E	185	44% 42% 13%
2	B	236	48% 42% 6%
2	F	236	50% 40% 9%
3	C	182	41% 51% 7%

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Mol	Chain	Length	Quality of chain
3	G	182	
4	D	217	
4	H	217	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12716 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 TCR 2W20 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1476	935	243	291	7			
1	E	184	Total	C	N	O	S	0	0	0
			1464	926	242	289	7			

- Molecule 2 is a protein called TCR 2W20 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1797	1129	319	343	6			
2	F	236	Total	C	N	O	S	0	0	0
			1870	1175	330	359	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			
3	G	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			

- Molecule 4 is a protein called 3K peptide, Linker,and H-2 class II histocompatibility antigen (A beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total	C	N	O	S	0	0	0
			1594	1002	288	297	7			
4	H	192	Total	C	N	O	S	0	0	0
			1594	1002	288	297	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	linker	UNP P14483
D	15	GLY	-	linker	UNP P14483
D	16	GLY	-	linker	UNP P14483
D	17	GLY	-	linker	UNP P14483
D	18	SER	-	linker	UNP P14483
D	19	LEU	-	linker	UNP P14483
D	20	VAL	-	linker	UNP P14483
D	21	PRO	-	linker	UNP P14483
D	22	ARG	-	linker	UNP P14483
D	23	GLY	-	linker	UNP P14483
D	24	SER	-	linker	UNP P14483
D	25	GLY	-	linker	UNP P14483
D	26	GLY	-	linker	UNP P14483
D	27	GLY	-	linker	UNP P14483
D	28	GLY	-	linker	UNP P14483
D	216	LYS	ARG	engineered mutation	UNP P14483
H	14	GLY	-	linker	UNP P14483
H	15	GLY	-	linker	UNP P14483
H	16	GLY	-	linker	UNP P14483
H	17	GLY	-	linker	UNP P14483
H	18	SER	-	linker	UNP P14483
H	19	LEU	-	linker	UNP P14483
H	20	VAL	-	linker	UNP P14483
H	21	PRO	-	linker	UNP P14483
H	22	ARG	-	linker	UNP P14483
H	23	GLY	-	linker	UNP P14483
H	24	SER	-	linker	UNP P14483
H	25	GLY	-	linker	UNP P14483
H	26	GLY	-	linker	UNP P14483
H	27	GLY	-	linker	UNP P14483
H	28	GLY	-	linker	UNP P14483
H	216	LYS	ARG	engineered mutation	UNP P14483

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

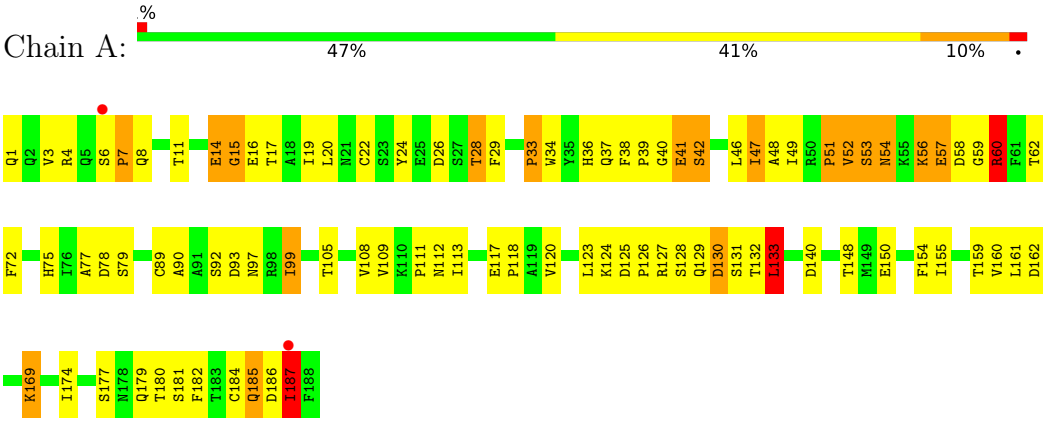
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	E	2	Total Ca 2 2	0	0

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 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.

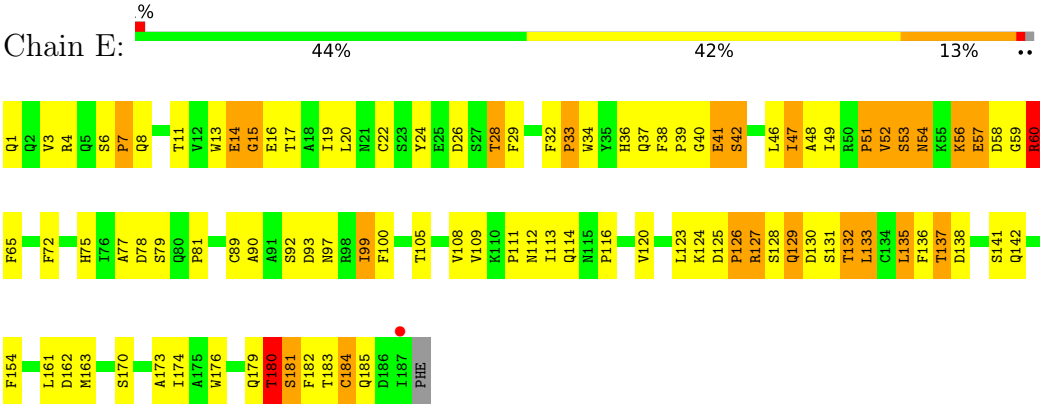
• Molecule 1: TCR 2W20 alpha chain

Chain A:



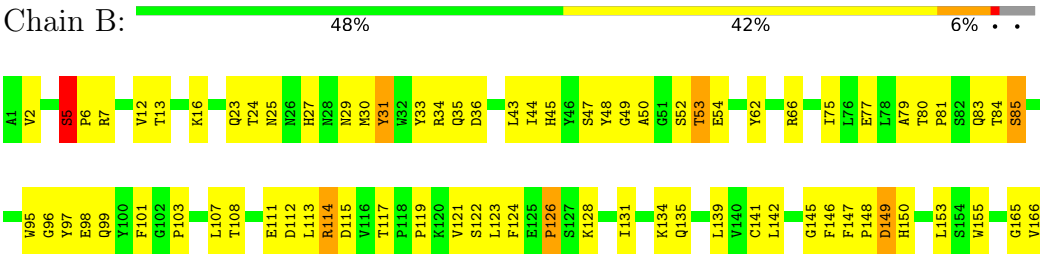
• Molecule 1: TCR 2W20 alpha chain

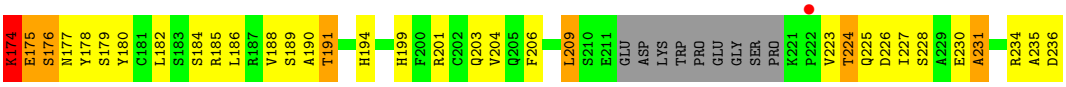
Chain E:



• Molecule 2: TCR 2W20 beta chain

Chain B:

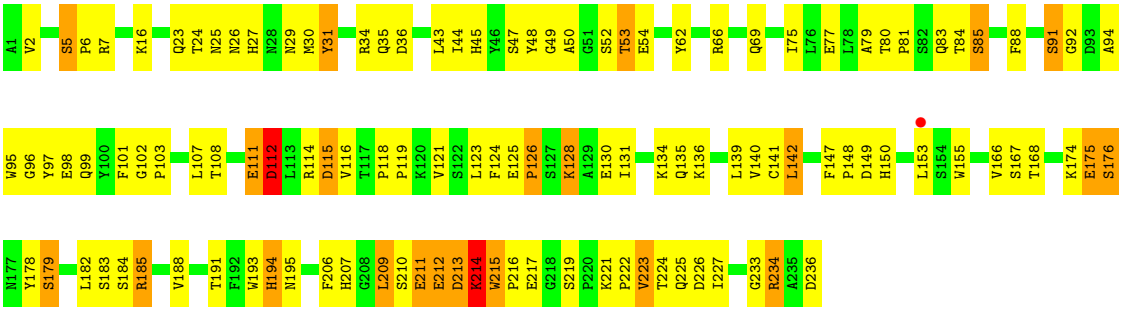




• Molecule 2: TCR 2W20 beta chain

Chain F:





• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

Chain C:

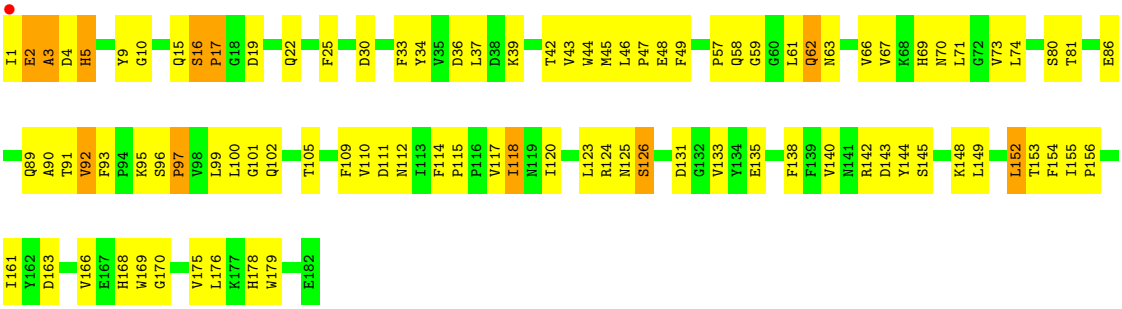




• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

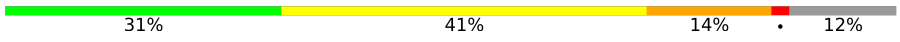
Chain G:



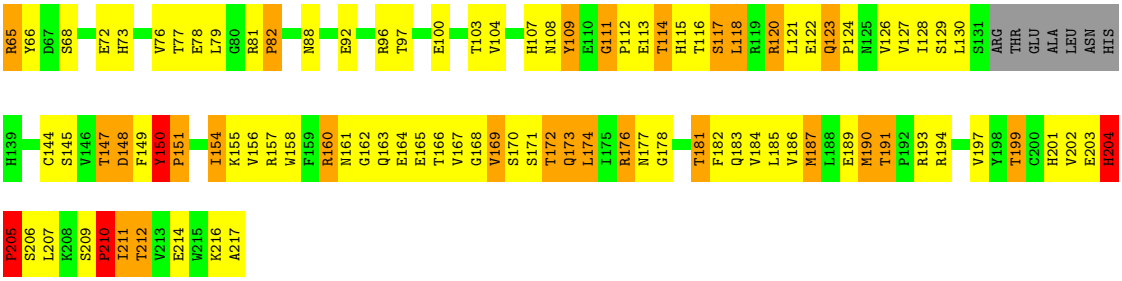


• Molecule 4: 3K peptide, Linker,and H-2 class II histocompatibility antigen (A beta chain)

Chain D:

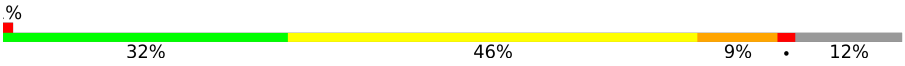


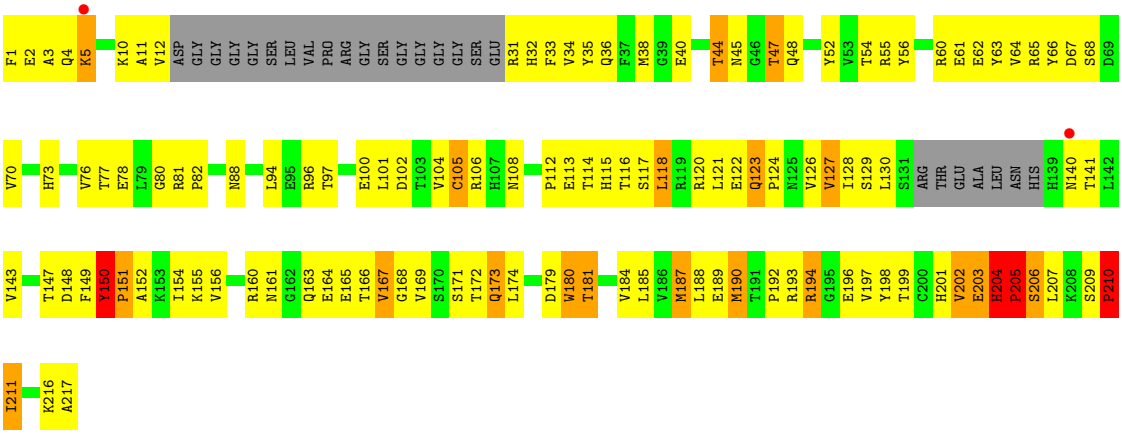




• Molecule 4: 3K peptide, Linker,and H-2 class II histocompatibility antigen (A beta chain)

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.54Å 113.93Å 386.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.40 49.07 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.07-3.40) 97.6 (49.07-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.325 0.258 , 0.311	Depositor DCC
R_{free} test set	1482 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	98.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 76.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12716	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.69	0/1514	1.03	5/2053 (0.2%)
1	E	0.61	0/1501	1.02	9/2037 (0.4%)
2	B	0.65	0/1847	1.04	7/2509 (0.3%)
2	F	0.62	0/1925	1.04	5/2618 (0.2%)
3	C	0.83	2/1504 (0.1%)	1.23	15/2054 (0.7%)
3	G	0.81	1/1504 (0.1%)	1.18	10/2054 (0.5%)
4	D	0.80	0/1632	1.28	21/2210 (1.0%)
4	H	0.78	0/1632	1.19	9/2210 (0.4%)
All	All	0.73	3/13059 (0.0%)	1.13	81/17745 (0.5%)

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
3	C	0	2
4	D	0	1
4	H	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	91	THR	CA-C	-5.34	1.47	1.53
3	C	73	VAL	CA-CB	-5.20	1.48	1.54
3	G	155	ILE	CA-CB	-5.08	1.49	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	205	PRO	N-CA-C	-9.68	102.29	114.68
4	D	150	TYR	CA-C-N	-9.18	108.36	119.84
4	D	150	TYR	C-N-CA	-9.18	108.36	119.84
1	A	187	ILE	N-CA-C	8.73	127.50	109.34
4	D	191	THR	CA-C-N	8.13	128.44	119.90
4	D	191	THR	C-N-CA	8.13	128.44	119.90
3	G	2	GLU	N-CA-C	8.01	121.79	110.50
3	C	107	ILE	N-CA-C	7.74	119.29	107.99
4	D	111	GLY	CA-C-N	7.36	126.90	119.24
4	D	111	GLY	C-N-CA	7.36	126.90	119.24
3	C	5	HIS	N-CA-C	7.27	126.29	110.80
4	D	187	MET	N-CA-C	7.14	119.19	110.41
3	G	118	ILE	N-CA-C	7.11	117.16	108.06
2	B	174	LYS	N-CA-C	7.08	125.88	110.80
1	A	28	THR	N-CA-C	-7.00	103.24	114.09
3	G	5	HIS	N-CA-C	6.99	125.68	110.80
4	D	204	HIS	N-CA-C	6.97	125.22	109.81
3	G	92	VAL	N-CA-C	6.88	118.56	109.21
4	D	6	ALA	N-CA-C	-6.85	99.80	110.42
3	C	45	MET	N-CA-C	-6.80	102.73	111.02
4	D	176	ARG	N-CA-C	-6.78	98.19	108.96
4	H	150	TYR	CA-C-N	-6.77	111.38	119.84
4	H	150	TYR	C-N-CA	-6.77	111.38	119.84
4	H	203	GLU	N-CA-C	6.68	120.29	109.40
3	G	145	SER	N-CA-C	-6.61	100.44	109.95
1	E	28	THR	N-CA-C	-6.47	104.05	114.09
4	H	204	HIS	N-CA-C	6.41	123.97	109.81
4	D	147	THR	N-CA-C	6.38	119.40	109.52
3	C	71	LEU	N-CA-C	-6.37	104.25	111.07
3	C	2	GLU	N-CA-C	6.37	124.36	110.80
4	H	147	THR	N-CA-C	6.33	118.92	108.99
2	F	101	PHE	N-CA-C	6.29	118.65	110.53
4	D	5	LYS	N-CA-C	6.27	119.63	110.17
2	B	173	TYR	N-CA-C	6.19	119.26	107.75
1	A	179	GLN	N-CA-C	6.09	119.16	108.75
1	E	184	CYS	CB-CA-C	-6.05	109.61	116.63
2	F	75	ILE	N-CA-C	6.00	116.65	107.77
3	C	159	ASP	N-CA-C	5.88	118.06	110.65
2	B	75	ILE	N-CA-C	5.83	116.40	107.77
1	E	179	GLN	N-CA-C	5.60	118.58	109.06
2	F	128	LYS	N-CA-C	-5.58	106.42	113.18
2	B	101	PHE	N-CA-C	5.57	117.72	110.53
4	D	65	ARG	N-CA-C	5.56	117.52	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	SER	CA-C-N	-5.52	112.94	119.84
2	B	5	SER	C-N-CA	-5.52	112.94	119.84
3	C	140	VAL	N-CA-C	5.48	117.46	108.97
1	E	42	SER	N-CA-C	5.47	117.44	109.84
1	E	99	ILE	N-CA-C	5.42	117.37	108.97
2	F	112	ASP	N-CA-C	-5.39	103.51	110.19
4	D	148	ASP	N-CA-C	5.36	118.64	111.24
2	B	111	GLU	N-CA-C	-5.36	104.33	111.24
3	G	9	TYR	N-CA-C	5.34	116.70	109.11
3	G	154	PHE	N-CA-C	5.33	116.37	108.86
3	C	137	SER	N-CA-C	-5.32	103.67	110.53
1	E	137	THR	N-CA-C	5.31	117.05	109.14
3	G	133	VAL	CB-CA-C	-5.30	104.55	111.81
1	E	183	THR	N-CA-C	5.30	120.22	113.18
4	D	60	ARG	N-CA-C	-5.29	104.55	112.54
3	C	174	PRO	CA-C-N	-5.27	117.96	122.96
3	C	174	PRO	C-N-CA	-5.27	117.96	122.96
4	H	202	VAL	N-CA-C	5.26	116.06	108.48
1	A	42	SER	N-CA-C	5.26	117.15	109.84
3	G	66	VAL	N-CA-C	-5.22	105.39	113.16
4	H	180	TRP	N-CA-C	5.21	118.78	111.74
1	A	99	ILE	N-CA-C	5.20	117.03	108.97
4	D	45	ASN	N-CA-C	-5.20	106.89	113.23
3	C	145	SER	N-CA-C	-5.17	102.25	109.69
4	D	145	SER	N-CA-C	5.17	117.66	109.96
1	E	135	LEU	N-CA-C	5.14	116.41	109.11
4	D	205	PRO	N-CA-C	-5.13	101.91	112.47
4	H	47	THR	N-CA-C	-5.11	105.51	112.26
1	E	126	PRO	N-CA-C	-5.08	108.11	114.20
3	G	16	SER	N-CA-C	5.08	119.41	112.55
3	C	16	SER	N-CA-C	5.08	121.03	109.81
4	D	160	ARG	CA-C-O	5.06	120.88	117.94
3	C	166	VAL	N-CA-C	5.04	114.83	107.37
2	F	185	ARG	N-CA-C	5.02	116.60	108.26
4	D	172	THR	N-CA-C	5.01	118.93	112.41
3	C	56	ASP	CA-C-N	5.00	125.28	119.47
3	C	56	ASP	C-N-CA	5.00	125.28	119.47
4	D	212	THR	N-CA-C	5.00	117.09	107.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	TYR	Sidechain
3	C	9	TYR	Sidechain
4	D	35	TYR	Sidechain
4	H	150	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1476	0	1402	94	0
1	E	1464	0	1394	108	0
2	B	1797	0	1703	127	0
2	F	1870	0	1765	137	0
3	C	1459	0	1386	123	0
3	G	1459	0	1386	106	0
4	D	1594	0	1534	175	0
4	H	1594	0	1534	163	0
5	A	1	0	0	0	0
5	E	2	0	0	0	0
All	All	12716	0	12104	916	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 37.

All (916) 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)
3:C:3:ALA:HB1	4:H:164:GLU:H	0.97	1.10
3:C:109:PHE:HE2	3:C:111:ASP:HB2	1.16	1.08
3:C:2:GLU:HA	4:D:45:ASN:OD1	1.55	1.05
3:C:71:LEU:HD23	4:D:35:TYR:HB2	1.40	1.03
4:H:116:THR:HG23	4:H:117:SER:H	1.17	1.02
3:G:15:GLN:HE22	3:G:117:VAL:HG23	1.25	1.02
2:B:7:ARG:HH21	2:B:103:PRO:HB2	1.23	1.00
4:D:5:LYS:H	4:D:5:LYS:HD3	1.27	1.00
2:F:5:SER:HB3	2:F:6:PRO:HD3	1.42	1.00
2:F:7:ARG:HH21	2:F:103:PRO:HB2	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:PRO:HG3	4:D:205:PRO:HA	1.41	0.98
1:A:99:ILE:HD12	2:B:99:GLN:HE21	1.29	0.97
3:C:3:ALA:HB1	4:H:164:GLU:N	1.78	0.96
4:D:52:TYR:H	4:D:68:SER:HB2	1.29	0.96
2:B:5:SER:HB3	2:B:6:PRO:HD3	1.44	0.95
2:F:147:PHE:HB3	2:F:148:PRO:HD3	1.50	0.94
4:D:151:PRO:HG3	4:D:205:PRO:CA	1.98	0.94
3:C:15:GLN:HG2	4:D:34:VAL:HG22	1.46	0.93
1:E:99:ILE:HD12	2:F:99:GLN:HE21	1.31	0.93
4:D:123:GLN:NE2	4:D:123:GLN:H	1.68	0.92
4:D:172:THR:O	4:D:173:GLN:HG2	1.69	0.92
3:G:71:LEU:HD23	4:H:35:TYR:HB2	1.54	0.90
4:H:172:THR:O	4:H:173:GLN:HB3	1.72	0.90
4:D:202:VAL:HB	4:D:211:ILE:HG23	1.54	0.89
1:E:124:LYS:HA	1:E:131:SER:HB3	1.55	0.89
1:A:123:LEU:HD23	1:A:133:LEU:HD12	1.56	0.88
3:C:2:GLU:HA	4:D:45:ASN:CG	1.98	0.88
4:H:202:VAL:HB	4:H:211:ILE:HG23	1.54	0.87
4:H:122:GLU:HB2	4:H:150:TYR:H	1.40	0.86
3:C:67:VAL:HG13	4:D:35:TYR:HD2	1.40	0.86
3:C:109:PHE:CE2	3:C:111:ASP:HB2	2.07	0.85
4:D:199:THR:HG23	4:D:214:GLU:HG3	1.59	0.84
4:H:4:GLN:HG3	4:H:5:LYS:H	1.42	0.84
3:C:46:LEU:O	3:C:49:PHE:HB2	1.77	0.84
3:G:15:GLN:HE22	3:G:117:VAL:CG2	1.90	0.84
2:B:121:VAL:HG12	2:B:227:ILE:HG22	1.59	0.84
1:E:28:THR:HG21	4:H:2:GLU:OE2	1.78	0.84
3:C:15:GLN:NE2	3:C:115:PRO:HB2	1.93	0.83
1:A:28:THR:HG21	4:D:2:GLU:OE2	1.79	0.83
4:H:101:LEU:O	4:H:105:CYS:HB2	1.80	0.82
3:C:67:VAL:HG13	4:D:35:TYR:CD2	2.14	0.82
1:E:99:ILE:HD12	2:F:99:GLN:NE2	1.96	0.81
4:D:147:THR:HG22	4:D:183:GLN:HG3	1.61	0.81
1:E:20:LEU:HD22	1:E:105:THR:HG21	1.60	0.80
4:H:116:THR:HG23	4:H:117:SER:N	1.97	0.80
3:G:1:ILE:O	4:H:45:ASN:HA	1.82	0.80
3:G:161:ILE:HG21	3:G:178:HIS:NE2	1.97	0.80
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.46	0.80
1:A:20:LEU:HD22	1:A:105:THR:HG21	1.63	0.79
4:D:112:PRO:O	4:D:116:THR:HG22	1.82	0.79
3:G:16:SER:HB2	3:G:71:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:HG3	1:E:60:ARG:HH11	1.48	0.79
3:C:99:LEU:HD23	3:C:102:GLN:OE1	1.82	0.79
2:F:48:TYR:OH	3:G:58:GLN:HG3	1.83	0.78
2:B:114:ARG:HB2	2:B:114:ARG:NH1	1.98	0.78
4:H:151:PRO:HG3	4:H:205:PRO:HA	1.64	0.78
4:D:52:TYR:H	4:D:68:SER:CB	1.97	0.77
1:A:99:ILE:HD12	2:B:99:GLN:NE2	1.98	0.77
1:A:154:PHE:CZ	2:B:175:GLU:HG2	2.19	0.77
1:A:148:THR:HG22	1:A:150:GLU:H	1.47	0.77
2:F:34:ARG:HB2	2:F:44:ILE:HD11	1.64	0.77
3:C:110:VAL:HG21	3:C:120:ILE:HD13	1.66	0.77
4:D:124:PRO:HD3	4:D:205:PRO:HG2	1.67	0.77
2:B:84:THR:HG23	2:B:108:THR:HA	1.67	0.76
1:A:113:ILE:HG13	1:A:140:ASP:HA	1.67	0.75
1:E:99:ILE:CD1	2:F:99:GLN:HE21	1.99	0.75
2:F:84:THR:HG23	2:F:108:THR:HA	1.68	0.75
2:B:34:ARG:HB2	2:B:44:ILE:HD11	1.68	0.75
2:B:147:PHE:HB3	2:B:148:PRO:HD3	1.67	0.75
1:A:148:THR:H	1:A:155:ILE:HD12	1.50	0.75
4:H:204:HIS:CG	4:H:204:HIS:O	2.39	0.75
4:D:96:ARG:HG3	4:D:96:ARG:HH11	1.49	0.74
1:E:19:ILE:HG22	1:E:75:HIS:ND1	2.02	0.74
4:D:123:GLN:H	4:D:123:GLN:HE21	1.33	0.74
2:F:5:SER:CB	2:F:6:PRO:HD3	2.15	0.74
2:F:147:PHE:HE1	2:F:178:TYR:HA	1.51	0.74
2:B:128:LYS:O	2:B:131:ILE:HG13	1.88	0.74
3:C:74:LEU:HD11	4:D:63:TYR:CE2	2.22	0.74
4:D:4:GLN:HG3	4:D:5:LYS:N	2.00	0.74
1:E:56:LYS:HG2	1:E:57:GLU:H	1.52	0.74
1:A:19:ILE:HG22	1:A:75:HIS:ND1	2.02	0.74
3:C:3:ALA:CB	4:H:164:GLU:H	1.90	0.73
1:A:99:ILE:CD1	2:B:99:GLN:HE21	2.00	0.73
4:H:202:VAL:HB	4:H:211:ILE:CG2	2.18	0.73
3:G:67:VAL:HG13	4:H:35:TYR:HD2	1.54	0.73
2:F:209:LEU:HB3	2:F:213:ASP:OD1	1.87	0.73
1:A:6:SER:HB3	1:A:7:PRO:HD3	1.69	0.73
2:B:5:SER:CB	2:B:6:PRO:HD3	2.16	0.73
1:E:6:SER:HB3	1:E:7:PRO:HD3	1.69	0.72
1:A:56:LYS:HG2	1:A:57:GLU:H	1.55	0.72
3:C:110:VAL:HG21	3:C:120:ILE:CD1	2.19	0.72
4:D:78:GLU:HG3	4:D:81:ARG:HD2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ASP:HB3	1:E:29:PHE:CE2	2.25	0.72
4:H:78:GLU:HG3	4:H:81:ARG:HD2	1.72	0.72
4:H:174:LEU:HD13	4:H:184:VAL:HB	1.69	0.72
4:D:149:PHE:HB2	4:D:151:PRO:HD2	1.71	0.72
3:G:97:PRO:HG3	4:H:127:VAL:HG11	1.71	0.72
3:C:180:GLU:HG3	3:C:182:GLU:HB2	1.71	0.71
2:F:31:TYR:HB3	2:F:43:LEU:HD11	1.72	0.71
4:H:5:LYS:HD3	4:H:5:LYS:N	2.05	0.71
2:B:113:LEU:HD13	2:B:113:LEU:O	1.90	0.71
2:F:191:THR:HA	2:F:194:HIS:NE2	2.05	0.71
3:G:90:ALA:HA	3:G:109:PHE:O	1.90	0.71
2:B:54:GLU:HG2	3:C:58:GLN:NE2	2.04	0.71
4:H:73:HIS:HB2	4:H:88:ASN:HD21	1.56	0.71
3:C:97:PRO:HG3	4:D:127:VAL:HG11	1.70	0.71
1:E:14:GLU:HG3	1:E:111:PRO:HA	1.71	0.71
4:D:160:ARG:NH2	4:D:163:GLN:OE1	2.23	0.71
2:F:5:SER:HB3	2:F:6:PRO:CD	2.20	0.71
2:F:54:GLU:HG2	3:G:58:GLN:NE2	2.06	0.71
2:B:121:VAL:HG12	2:B:227:ILE:CG2	2.21	0.70
4:D:4:GLN:HG3	4:D:5:LYS:H	1.57	0.70
4:H:197:VAL:HG12	4:H:216:LYS:HB3	1.71	0.70
1:E:161:LEU:HB2	2:F:185:ARG:HH12	1.54	0.70
3:G:118:ILE:HD11	3:G:166:VAL:HG13	1.73	0.70
1:A:26:ASP:HB3	1:A:29:PHE:CE2	2.27	0.70
1:A:51:PRO:O	1:A:52:VAL:HG23	1.91	0.70
4:D:113:GLU:O	4:D:115:HIS:N	2.24	0.70
1:E:28:THR:HB	4:H:4:GLN:HE22	1.56	0.70
4:H:116:THR:CG2	4:H:117:SER:H	1.99	0.70
3:C:172:GLU:OE2	3:C:173:GLU:HG2	1.92	0.69
2:F:213:ASP:HB3	2:F:221:LYS:HD2	1.74	0.69
1:E:52:VAL:HG12	1:E:52:VAL:O	1.91	0.69
2:F:97:TYR:C	2:F:98:GLU:HG3	2.18	0.69
3:G:2:GLU:HG3	4:H:45:ASN:ND2	2.07	0.69
4:H:112:PRO:O	4:H:116:THR:HG22	1.93	0.69
1:A:52:VAL:HG12	1:A:52:VAL:O	1.92	0.69
3:C:81:THR:O	4:D:33:PHE:CE1	2.46	0.69
4:H:96:ARG:HG3	4:H:96:ARG:HH11	1.57	0.69
4:D:117:SER:O	4:D:118:LEU:C	2.36	0.68
2:B:31:TYR:HB3	2:B:43:LEU:HD11	1.74	0.68
3:C:103:PRO:HG3	3:C:155:ILE:CD1	2.22	0.68
1:E:133:LEU:HD11	2:F:140:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:HB3	2:B:234:ARG:HH12	1.59	0.68
3:C:15:GLN:HE22	3:C:117:VAL:HG23	1.58	0.68
2:F:50:ALA:HA	2:F:66:ARG:HG3	1.76	0.68
4:H:63:TYR:CD2	4:H:64:VAL:HG23	2.29	0.68
4:D:126:VAL:HG21	4:D:202:VAL:HG21	1.76	0.67
2:F:141:CYS:HB2	2:F:155:TRP:CH2	2.29	0.67
4:D:164:GLU:N	3:G:3:ALA:HB1	2.09	0.67
4:D:202:VAL:HB	4:D:211:ILE:CG2	2.24	0.67
2:B:147:PHE:CB	2:B:148:PRO:HD3	2.23	0.67
2:B:199:HIS:HE1	2:B:230:GLU:HB2	1.59	0.67
2:B:50:ALA:HA	2:B:66:ARG:HG3	1.75	0.67
3:C:11:ILE:HB	3:C:24:THR:HG23	1.76	0.67
3:G:58:GLN:NE2	3:G:61:LEU:HD22	2.09	0.67
1:A:125:ASP:C	1:A:127:ARG:H	2.03	0.67
4:H:124:PRO:HG3	4:H:205:PRO:HG3	1.77	0.67
2:B:5:SER:HB3	2:B:6:PRO:CD	2.23	0.66
4:H:160:ARG:HH11	4:H:190:MET:HE1	1.60	0.66
4:D:35:TYR:OH	4:D:56:TYR:HB3	1.96	0.66
4:D:52:TYR:N	4:D:68:SER:HB2	2.07	0.66
1:E:51:PRO:O	1:E:52:VAL:HG23	1.94	0.66
1:E:148:THR:HG22	1:E:150:GLU:H	1.61	0.66
2:F:153:LEU:HD21	2:F:168:THR:HG21	1.76	0.66
4:H:124:PRO:HD3	4:H:205:PRO:HG2	1.78	0.66
2:B:114:ARG:HB2	2:B:114:ARG:HH11	1.60	0.66
3:G:70:ASN:O	3:G:71:LEU:C	2.37	0.66
4:D:158:TRP:HD1	4:D:169:VAL:HG12	1.61	0.66
4:D:43:PHE:O	4:H:163:GLN:NE2	2.23	0.66
2:B:191:THR:HA	2:B:194:HIS:NE2	2.10	0.66
3:C:61:LEU:HD12	3:C:61:LEU:H	1.61	0.66
2:B:97:TYR:C	2:B:98:GLU:HG3	2.19	0.65
3:G:34:TYR:CE1	3:G:43:VAL:HB	2.30	0.65
2:B:148:PRO:O	2:B:150:HIS:N	2.26	0.65
3:G:30:ASP:HB3	4:H:180:TRP:CE2	2.30	0.65
1:E:47:ILE:HB	1:E:63:ILE:HD11	1.79	0.65
2:F:128:LYS:HG3	2:F:131:ILE:HD11	1.78	0.65
3:C:133:VAL:HG22	3:C:152:LEU:HD23	1.79	0.65
2:F:147:PHE:HB3	2:F:148:PRO:CD	2.23	0.65
2:F:209:LEU:HB3	2:F:213:ASP:CG	2.22	0.65
2:B:48:TYR:CE1	3:C:62:GLN:HG2	2.32	0.65
4:H:4:GLN:HG3	4:H:5:LYS:N	2.10	0.64
4:D:5:LYS:H	4:D:5:LYS:CD	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:GLU:H	3:G:3:ALA:HB1	1.62	0.64
4:H:5:LYS:H	4:H:5:LYS:HD3	1.62	0.64
2:F:95:TRP:CH2	3:G:62:GLN:HB3	2.32	0.64
4:H:108:ASN:HA	4:H:112:PRO:HD2	1.78	0.64
2:B:153:LEU:HD22	2:B:182:LEU:HD21	1.78	0.64
2:B:139:LEU:HD12	2:B:139:LEU:H	1.63	0.64
3:G:109:PHE:HD1	3:G:149:LEU:HD21	1.62	0.64
4:H:151:PRO:HG3	4:H:205:PRO:CA	2.27	0.64
2:B:209:LEU:HD12	2:B:209:LEU:H	1.63	0.64
4:D:160:ARG:HG3	4:D:160:ARG:HH11	1.63	0.64
2:F:111:GLU:HG2	2:F:112:ASP:H	1.61	0.64
4:D:116:THR:HG23	4:D:117:SER:H	1.61	0.63
4:D:44:THR:O	4:D:45:ASN:HB2	1.99	0.63
4:D:65:ARG:HG2	4:D:66:TYR:N	2.12	0.63
2:F:7:ARG:HB3	2:F:7:ARG:NH1	2.13	0.63
2:F:147:PHE:CB	2:F:148:PRO:HD3	2.27	0.63
4:H:193:ARG:CB	4:H:193:ARG:HH11	2.11	0.63
2:F:126:PRO:HD2	2:F:193:TRP:CH2	2.33	0.63
2:B:7:ARG:NH1	2:B:7:ARG:HB3	2.13	0.63
1:E:28:THR:HG21	4:H:2:GLU:CD	2.23	0.62
1:E:182:PHE:CZ	1:E:184:CYS:SG	2.93	0.62
2:F:44:ILE:O	2:F:45:HIS:ND1	2.33	0.62
4:D:66:TYR:HB2	4:D:73:HIS:ND1	2.15	0.62
4:H:44:THR:O	4:H:45:ASN:HB2	1.98	0.62
3:C:15:GLN:HE21	3:C:115:PRO:HB2	1.64	0.62
3:C:16:SER:OG	4:D:33:PHE:HB2	1.99	0.62
3:C:98:VAL:HG13	3:C:156:PRO:HB3	1.82	0.62
3:G:161:ILE:CG2	3:G:178:HIS:NE2	2.62	0.62
2:F:134:LYS:O	2:F:135:GLN:HB2	2.00	0.62
2:F:193:TRP:CD1	2:F:193:TRP:C	2.78	0.62
3:G:138:PHE:CE1	3:G:148:LYS:HE2	2.35	0.62
3:C:90:ALA:HA	3:C:109:PHE:O	2.00	0.62
4:D:165:GLU:O	4:D:166:THR:HG23	2.00	0.62
1:A:174:ILE:HD11	2:B:185:ARG:HD2	1.81	0.62
3:C:97:PRO:O	3:C:99:LEU:HD22	1.99	0.61
4:D:173:GLN:CG	4:D:173:GLN:O	2.48	0.61
2:F:168:THR:HG23	2:F:184:SER:HB2	1.82	0.61
1:A:56:LYS:O	1:A:57:GLU:O	2.18	0.61
4:D:184:VAL:C	4:D:185:LEU:HD12	2.25	0.61
2:F:225:GLN:NE2	2:F:227:ILE:HD11	2.14	0.61
3:G:58:GLN:HE22	3:G:61:LEU:HD22	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.15	0.61
2:F:153:LEU:HD22	2:F:182:LEU:HD21	1.81	0.61
4:H:65:ARG:HG2	4:H:66:TYR:N	2.14	0.61
3:C:55:PHE:O	3:C:57:PRO:HD3	1.99	0.61
4:D:113:GLU:C	4:D:115:HIS:H	2.09	0.61
2:F:111:GLU:H	2:F:111:GLU:CD	2.09	0.61
4:H:122:GLU:HB2	4:H:150:TYR:N	2.15	0.61
4:H:160:ARG:HH11	4:H:160:ARG:HG3	1.66	0.61
4:H:165:GLU:O	4:H:166:THR:HG23	2.00	0.61
2:B:95:TRP:CH2	3:C:62:GLN:HB3	2.35	0.61
3:G:2:GLU:HA	4:H:45:ASN:CG	2.26	0.61
4:D:151:PRO:CG	4:D:205:PRO:HA	2.26	0.61
2:B:203:GLN:NE2	2:B:226:ASP:HB2	2.16	0.61
3:G:36:ASP:OD2	3:G:39:LYS:HE3	2.01	0.61
1:E:33:PRO:HG2	1:E:90:ALA:HB3	1.83	0.60
3:G:95:LYS:HE3	4:H:179:ASP:OD1	2.01	0.60
4:D:78:GLU:O	4:D:81:ARG:HG3	2.01	0.60
1:E:124:LYS:HA	1:E:131:SER:CB	2.30	0.60
2:B:49:GLY:O	2:B:52:SER:HB3	2.02	0.60
2:B:121:VAL:CG1	2:B:227:ILE:HG22	2.30	0.60
1:E:113:ILE:HD12	1:E:138:ASP:O	2.00	0.60
4:D:36:GLN:HB2	4:D:57:ILE:HB	1.82	0.60
3:G:123:LEU:HD22	3:G:126:SER:O	2.01	0.60
4:H:173:GLN:HG2	4:H:174:LEU:O	2.01	0.60
2:F:31:TYR:N	2:F:31:TYR:CD1	2.70	0.60
2:F:148:PRO:O	2:F:150:HIS:N	2.30	0.60
2:F:213:ASP:O	2:F:215:TRP:N	2.35	0.60
4:D:100:GLU:HA	4:D:103:THR:OG1	2.02	0.60
4:D:150:TYR:N	4:D:151:PRO:CD	2.65	0.60
4:D:116:THR:O	4:D:117:SER:O	2.20	0.60
4:D:160:ARG:HH11	4:D:190:MET:HE1	1.66	0.60
2:F:16:LYS:HZ1	2:F:77:GLU:HG3	1.67	0.60
2:F:209:LEU:HD12	2:F:222:PRO:HG2	1.84	0.60
2:B:153:LEU:HD22	2:B:182:LEU:CD2	2.31	0.59
3:G:46:LEU:O	3:G:47:PRO:C	2.44	0.59
1:A:124:LYS:HA	1:A:131:SER:HB3	1.83	0.59
1:E:46:LEU:HG	1:E:47:ILE:HG13	1.84	0.59
2:F:123:LEU:HD23	2:F:124:PHE:N	2.17	0.59
2:F:211:GLU:O	2:F:213:ASP:N	2.35	0.59
4:H:55:ARG:HG2	4:H:55:ARG:HH11	1.67	0.59
4:D:62:GLU:HG2	4:D:76:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LYS:HG2	1:E:57:GLU:N	2.17	0.59
3:G:16:SER:HB2	3:G:71:LEU:CD1	2.33	0.59
4:H:193:ARG:HH11	4:H:193:ARG:HB3	1.67	0.59
2:B:7:ARG:NH2	2:B:103:PRO:HB2	2.06	0.59
3:G:63:ASN:O	3:G:67:VAL:HG23	2.03	0.59
4:D:160:ARG:NH1	4:D:190:MET:HE1	2.17	0.59
3:G:120:ILE:HD12	3:G:148:LYS:HD2	1.83	0.59
1:A:125:ASP:OD1	1:A:131:SER:HA	2.02	0.59
2:B:134:LYS:O	2:B:135:GLN:HB2	2.01	0.59
3:C:33:PHE:HB2	3:C:43:VAL:O	2.02	0.59
3:G:89:GLN:O	3:G:110:VAL:HA	2.03	0.59
4:H:148:ASP:HA	4:H:181:THR:HB	1.85	0.59
3:C:118:ILE:HD11	3:C:166:VAL:HG13	1.84	0.59
2:B:119:PRO:O	2:B:227:ILE:HG13	2.02	0.59
3:C:103:PRO:HG3	3:C:155:ILE:HD11	1.84	0.59
1:E:135:LEU:O	1:E:135:LEU:HG	2.02	0.59
2:F:207:HIS:HA	2:F:224:THR:HG23	1.84	0.58
2:B:44:ILE:O	2:B:45:HIS:ND1	2.36	0.58
3:C:124:ARG:HG3	3:C:162:TYR:CE1	2.37	0.58
1:A:47:ILE:HB	1:A:63:ILE:HD11	1.83	0.58
4:D:173:GLN:O	4:D:173:GLN:HG3	2.03	0.58
1:E:60:ARG:HG3	1:E:60:ARG:NH1	2.17	0.58
4:H:143:VAL:HG22	4:H:187:MET:CG	2.33	0.58
4:H:189:GLU:HA	4:H:189:GLU:OE1	2.03	0.58
4:H:197:VAL:HG23	4:H:197:VAL:O	2.03	0.58
4:D:81:ARG:N	4:D:82:PRO:CD	2.66	0.58
1:E:56:LYS:O	1:E:57:GLU:O	2.21	0.58
3:G:17:PRO:HG3	4:H:32:HIS:HA	1.84	0.58
4:H:143:VAL:HG22	4:H:187:MET:HG3	1.85	0.58
4:D:122:GLU:HB2	4:D:150:TYR:H	1.68	0.58
3:G:15:GLN:HG2	4:H:34:VAL:HG22	1.84	0.58
3:G:46:LEU:HD23	3:G:49:PHE:CE1	2.39	0.58
2:B:31:TYR:CD1	2:B:31:TYR:N	2.72	0.58
4:H:197:VAL:HG12	4:H:216:LYS:CB	2.33	0.58
1:A:93:ASP:CG	1:A:97:ASN:H	2.11	0.58
2:B:225:GLN:HE21	2:B:227:ILE:HD11	1.69	0.58
4:D:96:ARG:HG3	4:D:96:ARG:NH1	2.17	0.58
4:D:160:ARG:HD2	4:D:161:ASN:N	2.18	0.58
2:F:7:ARG:NH2	2:F:103:PRO:HB2	2.10	0.58
1:A:53:SER:O	1:A:54:ASN:HB3	2.04	0.58
2:B:117:THR:HB	2:B:145:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:GLN:HE21	3:C:116:PRO:HD2	1.68	0.58
4:D:204:HIS:CG	4:D:204:HIS:O	2.53	0.58
3:C:16:SER:N	3:C:17:PRO:HD2	2.19	0.57
1:E:19:ILE:O	1:E:19:ILE:HG13	2.03	0.57
2:F:26:ASN:O	4:H:10:LYS:NZ	2.37	0.57
2:F:47:SER:HB3	2:F:66:ARG:HH11	1.69	0.57
2:B:153:LEU:H	2:B:153:LEU:HD23	1.69	0.57
4:D:160:ARG:HG3	4:D:160:ARG:NH1	2.19	0.57
1:A:56:LYS:HG2	1:A:57:GLU:N	2.20	0.57
2:B:47:SER:HB3	2:B:66:ARG:HH11	1.68	0.57
1:E:3:VAL:C	1:E:4:ARG:HD2	2.29	0.57
4:D:120:ARG:HG2	4:D:120:ARG:O	2.01	0.57
4:D:173:GLN:HA	4:H:169:VAL:O	2.04	0.57
1:A:17:THR:HG22	1:A:77:ALA:HA	1.86	0.57
3:C:16:SER:HB3	3:C:71:LEU:CD1	2.34	0.57
3:G:86:GLU:HG3	4:H:60:ARG:HH12	1.69	0.57
1:A:33:PRO:HG2	1:A:90:ALA:HB3	1.87	0.57
3:G:71:LEU:C	3:G:71:LEU:HD13	2.28	0.57
3:G:124:ARG:O	3:G:125:ASN:HB2	2.05	0.57
4:H:3:ALA:HB2	4:H:112:PRO:HG2	1.87	0.57
1:A:3:VAL:C	1:A:4:ARG:HD2	2.30	0.57
4:D:36:GLN:N	4:D:57:ILE:O	2.38	0.57
4:H:141:THR:HG23	4:H:188:LEU:O	2.04	0.57
3:C:118:ILE:HG13	3:C:167:GLU:O	2.05	0.57
3:C:151:TYR:OH	4:D:178:GLY:HA3	2.05	0.56
1:E:93:ASP:CG	1:E:97:ASN:H	2.12	0.56
2:F:49:GLY:O	2:F:52:SER:HB3	2.04	0.56
2:F:116:VAL:HG13	2:F:148:PRO:CD	2.34	0.56
2:B:23:GLN:HG2	2:B:24:THR:N	2.19	0.56
3:C:95:LYS:NZ	4:D:148:ASP:OD1	2.34	0.56
3:C:175:VAL:O	3:C:175:VAL:HG23	2.04	0.56
4:D:158:TRP:CD1	4:D:169:VAL:HG12	2.39	0.56
2:F:210:SER:O	2:F:211:GLU:C	2.48	0.56
3:G:109:PHE:HD1	3:G:149:LEU:CD2	2.19	0.56
4:D:114:THR:O	4:D:114:THR:HG22	2.04	0.56
1:E:53:SER:O	1:E:54:ASN:HB3	2.04	0.56
4:H:76:VAL:HG13	4:H:77:THR:HG23	1.88	0.56
1:E:49:ILE:HD13	1:E:65:PHE:HB2	1.87	0.56
4:H:52:TYR:H	4:H:68:SER:HB2	1.71	0.56
3:C:15:GLN:NE2	3:C:116:PRO:HD2	2.20	0.56
3:C:17:PRO:HG3	4:D:32:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LYS:HA	3:C:176:LEU:HA	1.86	0.56
1:E:174:ILE:HD11	2:F:185:ARG:HD2	1.87	0.56
4:H:193:ARG:HB2	4:H:196:GLU:OE2	2.05	0.56
1:A:46:LEU:HG	1:A:47:ILE:HG13	1.86	0.56
1:E:123:LEU:HD21	1:E:135:LEU:HB2	1.88	0.56
1:E:126:PRO:HD3	2:F:125:GLU:OE1	2.05	0.56
3:G:73:VAL:HG21	4:H:11:ALA:HB3	1.86	0.56
4:D:72:GLU:HB2	4:D:88:ASN:OD1	2.06	0.56
2:F:153:LEU:HD22	2:F:182:LEU:CD2	2.36	0.56
2:B:174:LYS:HD3	2:B:174:LYS:C	2.30	0.55
3:C:47:PRO:C	3:C:49:PHE:H	2.14	0.55
4:D:160:ARG:CD	4:D:161:ASN:H	2.19	0.55
4:D:187:MET:SD	4:D:187:MET:N	2.78	0.55
3:G:17:PRO:HG3	4:H:32:HIS:ND1	2.21	0.55
4:H:194:ARG:HG3	4:H:217:ALA:OXT	2.06	0.55
4:H:67:ASP:HB3	4:H:70:VAL:HG23	1.88	0.55
2:B:5:SER:CB	2:B:6:PRO:CD	2.83	0.55
4:D:63:TYR:CD2	4:D:64:VAL:HG23	2.41	0.55
2:F:16:LYS:NZ	2:F:77:GLU:HG3	2.21	0.55
3:G:74:LEU:HD21	4:H:63:TYR:OH	2.06	0.55
2:B:174:LYS:HD3	2:B:175:GLU:N	2.21	0.55
1:E:81:PRO:CG	1:E:111:PRO:HB3	2.37	0.55
4:D:81:ARG:NH1	4:D:81:ARG:HB3	2.22	0.55
4:D:216:LYS:HG2	4:D:217:ALA:H	1.70	0.55
1:E:20:LEU:CD2	1:E:105:THR:HG21	2.33	0.55
1:E:113:ILE:CD1	1:E:138:ASP:O	2.55	0.55
1:E:123:LEU:HD23	1:E:133:LEU:HD12	1.89	0.55
2:F:141:CYS:HB2	2:F:155:TRP:CZ2	2.42	0.55
1:A:49:ILE:HD13	1:A:65:PHE:HB2	1.89	0.55
2:B:165:GLY:O	2:B:186:LEU:HD12	2.07	0.55
3:C:86:GLU:HB3	3:C:112:ASN:HD21	1.72	0.55
2:F:147:PHE:CE1	2:F:178:TYR:HA	2.38	0.55
4:D:8:ALA:HB2	4:D:37:PHE:CD2	2.41	0.55
3:G:114:PHE:CD1	3:G:114:PHE:C	2.85	0.55
3:C:37:LEU:HD21	3:C:64:ILE:HG13	1.89	0.54
2:F:48:TYR:CE1	3:G:62:GLN:HG2	2.42	0.54
3:G:16:SER:HB3	4:H:33:PHE:HB2	1.90	0.54
4:D:51:ARG:HG3	4:D:68:SER:HB3	1.89	0.54
2:F:23:GLN:HG2	2:F:24:THR:N	2.21	0.54
1:A:161:LEU:HB2	2:B:185:ARG:HH12	1.72	0.54
2:B:128:LYS:HA	2:B:131:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:GLU:HB3	3:C:112:ASN:ND2	2.23	0.54
2:F:5:SER:CB	2:F:6:PRO:CD	2.81	0.54
4:H:150:TYR:CG	4:H:150:TYR:O	2.59	0.54
1:A:19:ILE:HG13	1:A:19:ILE:O	2.07	0.54
3:C:2:GLU:O	3:C:3:ALA:O	2.26	0.54
3:G:42:THR:OG1	3:G:57:PRO:HG3	2.07	0.54
2:B:199:HIS:CE1	2:B:230:GLU:HB2	2.42	0.54
2:F:147:PHE:HD1	2:F:179:SER:H	1.55	0.54
2:B:148:PRO:C	2:B:150:HIS:H	2.13	0.54
3:C:136:THR:O	3:C:148:LYS:NZ	2.40	0.54
4:D:216:LYS:O	4:D:217:ALA:HB3	2.08	0.54
4:D:120:ARG:HD3	4:D:150:TYR:CD1	2.44	0.54
3:G:2:GLU:HG3	4:H:45:ASN:HD21	1.73	0.54
1:A:36:HIS:O	1:A:36:HIS:ND1	2.41	0.53
4:D:172:THR:O	4:D:173:GLN:CG	2.49	0.53
4:H:188:LEU:HD12	4:H:189:GLU:N	2.24	0.53
1:E:123:LEU:HD12	2:F:126:PRO:HA	1.89	0.53
3:G:81:THR:O	4:H:33:PHE:HE1	1.91	0.53
4:H:160:ARG:NH1	4:H:190:MET:HE1	2.23	0.53
1:A:123:LEU:HD12	2:B:126:PRO:HA	1.89	0.53
2:B:16:LYS:NZ	2:B:77:GLU:HG3	2.23	0.53
2:B:16:LYS:HD2	2:B:77:GLU:HA	1.91	0.53
2:F:118:PRO:HD3	2:F:222:PRO:HB3	1.91	0.53
2:F:123:LEU:HD23	2:F:123:LEU:C	2.33	0.53
2:F:168:THR:HG23	2:F:183:SER:O	2.09	0.53
2:B:146:PHE:CE1	2:B:180:TYR:O	2.62	0.53
4:D:122:GLU:HB2	4:D:150:TYR:N	2.24	0.53
3:C:37:LEU:N	3:C:37:LEU:HD12	2.24	0.53
2:B:199:HIS:HE1	2:B:230:GLU:CB	2.22	0.52
2:F:94:ALA:CB	3:G:62:GLN:HE22	2.22	0.52
1:A:33:PRO:HA	1:A:48:ALA:HA	1.91	0.52
2:B:16:LYS:HZ1	2:B:77:GLU:HG3	1.74	0.52
4:D:176:ARG:HG3	4:D:182:PHE:HE1	1.73	0.52
3:G:15:GLN:HE21	3:G:115:PRO:HB2	1.74	0.52
3:G:33:PHE:HB2	3:G:43:VAL:O	2.10	0.52
4:D:124:PRO:HG3	4:D:205:PRO:HG3	1.91	0.52
4:D:76:VAL:HG13	4:D:77:THR:HG23	1.92	0.52
1:E:33:PRO:HA	1:E:48:ALA:HA	1.91	0.52
2:F:94:ALA:HB1	3:G:62:GLN:NE2	2.25	0.52
2:B:123:LEU:HD23	2:B:123:LEU:C	2.35	0.52
2:F:29:ASN:HB2	2:F:92:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:N	1:A:174:ILE:HD12	2.24	0.52
2:B:204:VAL:HG12	2:B:204:VAL:O	2.09	0.52
3:G:36:ASP:OD2	3:G:39:LYS:CE	2.58	0.52
4:D:201:HIS:NE2	4:D:210:PRO:HB3	2.25	0.52
4:D:207:LEU:HD23	4:D:207:LEU:N	2.24	0.52
1:E:163:MET:HE1	2:F:188:VAL:HA	1.92	0.52
2:F:16:LYS:HD2	2:F:77:GLU:HA	1.91	0.52
2:F:27:HIS:ND1	2:F:91:SER:OG	2.42	0.52
4:H:150:TYR:O	4:H:150:TYR:CD1	2.63	0.52
4:H:188:LEU:HD12	4:H:189:GLU:H	1.75	0.52
2:B:189:SER:O	2:B:190:ALA:C	2.53	0.52
3:C:119:ASN:HD22	3:C:167:GLU:CD	2.17	0.52
4:D:100:GLU:HB3	4:D:104:VAL:CG2	2.40	0.51
4:D:148:ASP:HA	4:D:181:THR:HB	1.91	0.51
4:D:162:GLY:O	3:G:3:ALA:HB2	2.10	0.51
2:F:209:LEU:HD13	2:F:213:ASP:OD2	2.10	0.51
3:C:98:VAL:HG13	3:C:156:PRO:CB	2.41	0.51
4:D:160:ARG:HD2	4:D:161:ASN:H	1.73	0.51
1:E:36:HIS:O	1:E:36:HIS:ND1	2.43	0.51
4:H:189:GLU:O	4:H:190:MET:O	2.28	0.51
1:A:165:ALA:O	1:A:166:MET:C	2.52	0.51
4:D:128:ILE:HG22	4:D:129:SER:N	2.25	0.51
1:E:36:HIS:HD2	1:E:46:LEU:HB2	1.76	0.51
4:H:88:ASN:OD1	4:H:94:LEU:HD13	2.10	0.51
2:B:113:LEU:HD11	2:B:209:LEU:CD2	2.41	0.51
3:C:81:THR:O	4:D:33:PHE:HE1	1.92	0.51
4:D:38:MET:HE2	4:D:40:GLU:OE2	2.11	0.51
4:D:124:PRO:CD	4:D:205:PRO:HG2	2.40	0.51
4:D:163:GLN:HA	3:G:3:ALA:HB1	1.91	0.51
4:D:170:SER:HB2	4:D:187:MET:HB2	1.92	0.51
4:D:171:SER:HB2	4:H:171:SER:HB3	1.93	0.51
3:G:15:GLN:HA	4:H:33:PHE:O	2.09	0.51
3:G:178:HIS:CD2	3:G:179:TRP:H	2.28	0.51
4:D:38:MET:CE	4:D:40:GLU:CD	2.84	0.51
4:D:144:CYS:HB2	4:D:158:TRP:CZ2	2.46	0.51
3:C:34:TYR:CE1	3:C:43:VAL:HB	2.46	0.51
1:E:4:ARG:O	1:E:22:CYS:HA	2.10	0.51
4:H:47:THR:HG22	4:H:106:ARG:HH12	1.76	0.51
4:H:120:ARG:HG3	4:H:120:ARG:HH11	1.75	0.51
4:D:79:LEU:HG	4:D:79:LEU:O	2.10	0.50
3:G:143:ASP:OD2	3:G:143:ASP:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:C	1:A:127:ARG:N	2.68	0.50
2:B:121:VAL:HG22	2:B:122:SER:N	2.25	0.50
3:C:124:ARG:O	3:C:125:ASN:HB2	2.12	0.50
2:B:36:ASP:OD2	2:B:85:SER:CB	2.59	0.50
4:D:197:VAL:O	4:D:197:VAL:HG23	2.12	0.50
2:B:153:LEU:HD23	2:B:153:LEU:N	2.27	0.50
3:C:123:LEU:HD23	3:C:128:SER:HA	1.93	0.50
4:D:4:GLN:CG	4:D:5:LYS:N	2.72	0.50
3:G:135:GLU:CD	3:G:148:LYS:HD3	2.36	0.50
4:D:62:GLU:OE1	4:D:65:ARG:NE	2.40	0.50
4:D:207:LEU:HD23	4:D:207:LEU:H	1.77	0.50
3:G:176:LEU:HD12	3:G:176:LEU:O	2.11	0.50
4:D:2:GLU:O	4:D:107:HIS:HE1	1.94	0.50
4:H:160:ARG:HG3	4:H:160:ARG:NH1	2.25	0.50
2:F:128:LYS:HD3	2:F:236:ASP:HB3	1.92	0.50
3:G:95:LYS:HZ3	4:H:148:ASP:CG	2.20	0.50
4:H:193:ARG:CB	4:H:193:ARG:NH1	2.74	0.50
4:H:193:ARG:HB2	4:H:193:ARG:NH1	2.27	0.50
1:A:92:SER:HB2	1:A:99:ILE:HG12	1.93	0.50
2:B:48:TYR:HE2	3:C:58:GLN:HE21	1.60	0.50
2:B:153:LEU:CD2	2:B:182:LEU:HD21	2.41	0.50
4:D:116:THR:HG23	4:D:117:SER:N	2.27	0.50
4:D:189:GLU:O	4:D:190:MET:C	2.54	0.50
1:E:92:SER:HB2	1:E:99:ILE:HG12	1.93	0.50
3:G:61:LEU:HD12	3:G:61:LEU:H	1.76	0.50
3:C:33:PHE:CD1	3:C:33:PHE:C	2.90	0.49
2:F:128:LYS:HD3	2:F:236:ASP:CG	2.36	0.49
3:G:168:HIS:CD2	3:G:170:GLY:H	2.29	0.49
2:B:79:ALA:HA	2:B:83:GLN:OE1	2.12	0.49
4:D:113:GLU:C	4:D:115:HIS:N	2.68	0.49
1:A:177:SER:OG	1:A:182:PHE:HD2	1.95	0.49
3:C:16:SER:HB3	3:C:71:LEU:HD11	1.93	0.49
4:H:190:MET:CE	4:H:198:TYR:HE2	2.26	0.49
4:H:190:MET:HE2	4:H:198:TYR:HE2	1.77	0.49
1:A:11:THR:HG22	1:A:108:VAL:HB	1.93	0.49
2:B:27:HIS:ND1	2:B:91:SER:OG	2.44	0.49
4:H:156:VAL:HA	4:H:201:HIS:O	2.13	0.49
2:B:203:GLN:HE21	2:B:226:ASP:HB2	1.77	0.49
4:D:174:LEU:HD13	4:D:184:VAL:HB	1.95	0.49
2:F:114:ARG:HG2	2:F:215:TRP:CZ2	2.48	0.49
4:H:126:VAL:HG21	4:H:202:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:GLU:OE2	2:F:234:ARG:NH2	2.46	0.49
3:C:151:TYR:CD1	3:C:151:TYR:N	2.81	0.49
3:C:180:GLU:CG	3:C:182:GLU:HB2	2.42	0.49
2:F:175:GLU:O	2:F:176:SER:HB3	2.11	0.49
1:A:20:LEU:CD2	1:A:105:THR:HG21	2.38	0.49
2:B:29:ASN:HB2	2:B:92:GLY:O	2.11	0.49
4:D:168:GLY:HA2	4:H:173:GLN:HG3	1.95	0.49
1:E:17:THR:HG22	1:E:77:ALA:HA	1.94	0.49
2:F:35:GLN:NE2	2:F:88:PHE:HE2	2.11	0.49
4:D:5:LYS:HD3	4:D:5:LYS:N	2.06	0.49
1:A:4:ARG:O	1:A:22:CYS:HA	2.13	0.49
4:D:167:VAL:HG23	4:D:168:GLY:N	2.28	0.49
3:G:33:PHE:CD1	3:G:33:PHE:C	2.90	0.49
3:C:17:PRO:HG3	4:D:32:HIS:HA	1.94	0.48
2:B:206:PHE:O	2:B:224:THR:HA	2.13	0.48
1:E:28:THR:CB	4:H:4:GLN:HE22	2.23	0.48
3:G:96:SER:HB3	3:G:97:PRO:HD2	1.95	0.48
1:A:93:ASP:OD2	1:A:97:ASN:N	2.43	0.48
3:C:15:GLN:NE2	3:C:116:PRO:CD	2.76	0.48
3:C:106:LEU:HB2	3:C:154:PHE:CE1	2.48	0.48
4:D:45:ASN:HB2	4:D:48:GLN:HB3	1.94	0.48
4:D:120:ARG:HG3	4:D:120:ARG:HH11	1.77	0.48
1:E:161:LEU:HD13	1:E:161:LEU:C	2.39	0.48
4:H:81:ARG:HB2	4:H:82:PRO:HD3	1.95	0.48
1:A:184:CYS:O	1:A:185:GLN:HB2	2.13	0.48
2:B:174:LYS:HA	2:B:180:TYR:HD1	1.77	0.48
3:C:22:GLN:HE21	3:C:24:THR:HG22	1.77	0.48
2:F:79:ALA:HA	2:F:83:GLN:OE1	2.13	0.48
2:F:121:VAL:HG12	2:F:227:ILE:HG22	1.95	0.48
4:H:160:ARG:HD2	4:H:161:ASN:ND2	2.28	0.48
4:H:172:THR:OG1	4:H:185:LEU:HB2	2.14	0.48
1:E:11:THR:HG22	1:E:108:VAL:HB	1.95	0.48
1:A:15:GLY:HA2	1:A:78:ASP:HA	1.95	0.48
4:D:203:GLU:O	4:D:205:PRO:HD3	2.14	0.48
3:C:69:HIS:HD2	4:D:10:LYS:HG3	1.78	0.48
3:C:129:VAL:HG22	3:C:130:ALA:N	2.29	0.48
4:H:54:THR:OG1	4:H:66:TYR:HB3	2.13	0.48
3:G:22:GLN:HE22	3:G:138:PHE:HB2	1.79	0.48
1:A:38:PHE:C	1:A:40:GLY:H	2.22	0.47
2:B:147:PHE:HB3	2:B:148:PRO:CD	2.40	0.47
2:F:23:GLN:HG2	2:F:25:ASN:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:53:THR:O	2:F:53:THR:HG23	2.14	0.47
2:F:114:ARG:NH2	2:F:215:TRP:CZ3	2.82	0.47
2:F:119:PRO:HD3	2:F:206:PHE:CD2	2.49	0.47
3:G:105:THR:HA	3:G:153:THR:HA	1.96	0.47
1:A:177:SER:OG	1:A:182:PHE:CD2	2.68	0.47
2:B:147:PHE:CE1	2:B:178:TYR:HA	2.47	0.47
2:B:184:SER:OG	2:B:185:ARG:N	2.44	0.47
3:C:93:PHE:O	3:C:106:LEU:HD12	2.14	0.47
4:D:100:GLU:HB3	4:D:104:VAL:HG21	1.96	0.47
2:F:209:LEU:HB3	2:F:213:ASP:OD2	2.15	0.47
2:B:194:HIS:HB2	2:B:235:ALA:HA	1.96	0.47
3:C:92:VAL:HG12	3:C:93:PHE:N	2.29	0.47
4:D:114:THR:O	4:D:114:THR:CG2	2.62	0.47
1:E:174:ILE:HD12	1:E:174:ILE:N	2.29	0.47
1:A:126:PRO:HB3	2:B:234:ARG:NH1	2.27	0.47
3:C:114:PHE:CZ	4:D:60:ARG:HG3	2.49	0.47
1:E:81:PRO:HG2	1:E:111:PRO:HB3	1.95	0.47
3:G:69:HIS:CD2	4:H:10:LYS:HG3	2.49	0.47
2:F:84:THR:O	2:F:85:SER:HB3	2.15	0.47
2:B:201:ARG:HD3	2:B:228:SER:OG	2.14	0.47
3:C:69:HIS:CD2	4:D:10:LYS:HG3	2.50	0.47
2:B:23:GLN:HG2	2:B:25:ASN:H	1.78	0.47
2:B:119:PRO:HG3	2:B:204:VAL:HG11	1.97	0.47
3:C:176:LEU:HD23	3:C:176:LEU:H	1.79	0.47
1:E:14:GLU:C	1:E:16:GLU:H	2.23	0.47
2:F:36:ASP:OD2	2:F:85:SER:CB	2.62	0.47
2:F:223:VAL:O	2:F:224:THR:C	2.56	0.47
4:D:37:PHE:HA	4:D:55:ARG:O	2.15	0.47
4:D:73:HIS:CE1	4:D:97:THR:HG21	2.50	0.47
4:D:165:GLU:O	4:D:166:THR:CG2	2.62	0.47
4:H:172:THR:O	4:H:173:GLN:CB	2.50	0.47
2:B:128:LYS:HA	2:B:131:ILE:CG1	2.45	0.47
2:B:153:LEU:H	2:B:153:LEU:CD2	2.28	0.47
2:B:174:LYS:HE2	2:B:176:SER:H	1.80	0.47
2:B:206:PHE:CD1	2:B:206:PHE:C	2.93	0.47
1:E:15:GLY:HA2	1:E:78:ASP:OD1	2.14	0.47
2:F:34:ARG:CB	2:F:44:ILE:HD11	2.41	0.47
2:F:123:LEU:HD21	2:F:139:LEU:HD23	1.96	0.47
3:C:106:LEU:HB2	3:C:154:PHE:CD1	2.50	0.46
3:G:101:GLY:H	3:G:156:PRO:HG2	1.79	0.46
4:H:100:GLU:O	4:H:104:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ARG:NH1	2:B:62:TYR:OH	2.47	0.46
3:C:119:ASN:ND2	3:C:167:GLU:OE2	2.47	0.46
4:D:165:GLU:C	4:D:166:THR:HG23	2.40	0.46
1:E:120:VAL:O	1:E:120:VAL:HG12	2.15	0.46
4:H:56:TYR:CD1	4:H:56:TYR:N	2.83	0.46
1:A:15:GLY:HA2	1:A:78:ASP:OD1	2.16	0.46
3:C:77:ARG:NH2	4:D:79:LEU:O	2.46	0.46
4:D:151:PRO:HG3	4:D:205:PRO:C	2.38	0.46
4:D:156:VAL:HG11	4:D:186:VAL:HG21	1.98	0.46
2:F:94:ALA:CB	3:G:62:GLN:NE2	2.78	0.46
2:F:153:LEU:HD11	2:F:184:SER:HB2	1.98	0.46
3:G:2:GLU:HA	4:H:45:ASN:OD1	2.15	0.46
4:H:81:ARG:N	4:H:82:PRO:CD	2.78	0.46
4:H:113:GLU:HA	4:H:116:THR:HG22	1.97	0.46
1:A:38:PHE:O	1:A:40:GLY:N	2.49	0.46
3:C:25:PHE:CG	3:C:33:PHE:CZ	3.03	0.46
3:C:165:LYS:HG3	3:C:165:LYS:O	2.15	0.46
4:D:193:ARG:O	4:D:194:ARG:C	2.58	0.46
2:F:114:ARG:CZ	2:F:215:TRP:CZ3	2.98	0.46
4:H:47:THR:HG22	4:H:47:THR:O	2.15	0.46
1:A:113:ILE:HB	1:A:140:ASP:CG	2.41	0.46
1:A:130:ASP:OD1	1:A:130:ASP:O	2.34	0.46
2:B:153:LEU:HD21	2:B:168:THR:HG21	1.97	0.46
3:C:124:ARG:HG3	3:C:162:TYR:HE1	1.79	0.46
1:E:125:ASP:OD1	1:E:131:SER:HA	2.15	0.46
4:H:189:GLU:O	4:H:190:MET:C	2.58	0.46
2:B:84:THR:HG23	2:B:107:LEU:O	2.15	0.46
3:G:69:HIS:NE2	4:H:10:LYS:HE3	2.30	0.46
4:H:52:TYR:H	4:H:68:SER:CB	2.28	0.46
2:B:84:THR:O	2:B:85:SER:HB3	2.16	0.46
3:C:163:ASP:HB3	3:C:176:LEU:HD12	1.98	0.46
4:D:123:GLN:NE2	4:D:123:GLN:N	2.50	0.46
2:F:114:ARG:CD	2:F:114:ARG:H	2.29	0.46
4:H:55:ARG:HG2	4:H:55:ARG:NH1	2.30	0.46
1:A:177:SER:HG	1:A:182:PHE:HD2	1.61	0.46
4:D:92:GLU:O	4:D:96:ARG:HB2	2.16	0.46
4:H:193:ARG:O	4:H:194:ARG:C	2.59	0.46
4:D:108:ASN:O	4:D:109:TYR:C	2.58	0.46
1:A:120:VAL:HG12	1:A:120:VAL:O	2.15	0.46
2:B:35:GLN:NE2	2:B:88:PHE:HE2	2.13	0.46
2:B:84:THR:HG21	2:B:108:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LEU:HD11	2:B:209:LEU:HD21	1.96	0.46
1:E:97:ASN:OD1	3:G:59:GLY:HA2	2.15	0.46
1:E:137:THR:OG1	1:E:138:ASP:N	2.49	0.46
1:A:64:PHE:CD1	1:A:75:HIS:HD2	2.34	0.45
2:B:121:VAL:HA	2:B:142:LEU:O	2.15	0.45
2:B:141:CYS:HB2	2:B:155:TRP:CZ2	2.51	0.45
4:D:111:GLY:HA3	4:D:112:PRO:HD3	1.81	0.45
1:E:13:TRP:HH2	1:E:142:GLN:N	2.14	0.45
1:E:33:PRO:HD2	1:E:90:ALA:O	2.15	0.45
2:F:174:LYS:HG2	2:F:175:GLU:N	2.31	0.45
1:A:112:ASN:CG	1:A:112:ASN:O	2.60	0.45
1:E:136:PHE:HB3	1:E:173:ALA:HB3	1.98	0.45
3:C:64:ILE:HD13	3:C:64:ILE:HA	1.73	0.45
4:H:12:VAL:O	4:H:12:VAL:HG12	2.16	0.45
1:A:117:GLU:O	1:A:117:GLU:HG2	2.17	0.45
1:E:28:THR:CG2	4:H:2:GLU:CD	2.90	0.45
1:E:123:LEU:N	1:E:123:LEU:HD22	2.32	0.45
2:F:34:ARG:NH1	2:F:62:TYR:OH	2.48	0.45
2:F:48:TYR:HE2	3:G:58:GLN:HE21	1.63	0.45
1:A:47:ILE:N	1:A:47:ILE:HD12	2.32	0.45
1:A:51:PRO:O	1:A:52:VAL:CG2	2.63	0.45
2:B:48:TYR:OH	3:C:58:GLN:HG3	2.17	0.45
3:C:88:PRO:HD3	3:C:168:HIS:HD2	1.81	0.45
1:E:38:PHE:C	1:E:40:GLY:H	2.25	0.45
1:A:37:GLN:HE22	2:B:35:GLN:HE22	1.65	0.45
3:C:118:ILE:HD11	3:C:166:VAL:CG1	2.47	0.45
3:C:172:GLU:CD	3:C:172:GLU:H	2.25	0.45
4:H:160:ARG:HG3	4:H:190:MET:HE2	1.99	0.45
2:B:80:THR:HB	2:B:81:PRO:HD2	1.99	0.45
2:B:148:PRO:C	2:B:150:HIS:N	2.74	0.45
4:D:52:TYR:O	4:D:68:SER:N	2.49	0.45
3:G:16:SER:N	3:G:17:PRO:HD2	2.31	0.45
1:E:15:GLY:HA2	1:E:78:ASP:HA	1.98	0.45
1:E:47:ILE:CG2	1:E:57:GLU:HB3	2.46	0.45
1:E:62:THR:OG1	1:E:75:HIS:HB2	2.17	0.45
3:G:30:ASP:HB3	4:H:180:TRP:NE1	2.32	0.45
4:H:150:TYR:N	4:H:151:PRO:CD	2.79	0.45
4:H:167:VAL:HG23	4:H:168:GLY:H	1.81	0.45
1:A:64:PHE:O	1:A:72:PHE:HA	2.16	0.45
1:A:186:ASP:C	1:A:187:ILE:HG12	2.41	0.45
3:C:99:LEU:O	3:C:100:LEU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:VAL:HG12	1:E:4:ARG:N	2.32	0.45
2:F:114:ARG:NH1	2:F:215:TRP:CH2	2.85	0.45
3:G:144:TYR:CE1	4:H:62:GLU:HB2	2.52	0.45
4:H:169:VAL:O	4:H:169:VAL:HG23	2.16	0.45
1:A:16:GLU:HG2	1:A:17:THR:N	2.32	0.44
1:A:47:ILE:CG2	1:A:57:GLU:HB3	2.47	0.44
3:C:13:VAL:HG12	3:C:14:TYR:N	2.32	0.44
3:C:47:PRO:C	3:C:49:PHE:N	2.75	0.44
4:D:209:SER:O	4:D:210:PRO:C	2.60	0.44
1:E:93:ASP:OD2	1:E:97:ASN:N	2.48	0.44
1:E:131:SER:O	1:E:132:THR:C	2.58	0.44
4:H:47:THR:CG2	4:H:106:ARG:NH1	2.80	0.44
4:H:121:LEU:O	4:H:122:GLU:HG2	2.17	0.44
4:H:209:SER:O	4:H:210:PRO:C	2.60	0.44
1:A:28:THR:HG21	4:D:2:GLU:CD	2.41	0.44
2:B:34:ARG:CB	2:B:44:ILE:HD11	2.43	0.44
3:C:119:ASN:HB2	3:C:167:GLU:HB3	1.98	0.44
4:D:63:TYR:CE2	4:D:64:VAL:HG23	2.53	0.44
4:H:130:LEU:HD23	4:H:140:ASN:HB2	1.99	0.44
3:C:73:VAL:HG12	3:C:77:ARG:HD3	1.99	0.44
3:C:151:TYR:HH	4:D:178:GLY:HA3	1.82	0.44
1:E:24:TYR:C	1:E:24:TYR:CD1	2.96	0.44
1:E:38:PHE:O	1:E:40:GLY:N	2.50	0.44
2:F:80:THR:HB	2:F:81:PRO:HD2	1.98	0.44
4:H:73:HIS:HB2	4:H:88:ASN:ND2	2.29	0.44
1:A:14:GLU:C	1:A:16:GLU:H	2.25	0.44
3:C:93:PHE:HB2	3:C:94:PRO:HD2	1.99	0.44
3:G:15:GLN:NE2	3:G:117:VAL:CG2	2.71	0.44
3:C:3:ALA:O	3:C:4:ASP:OD2	2.36	0.44
4:D:116:THR:O	4:D:117:SER:C	2.60	0.44
4:D:177:ASN:HD22	4:D:177:ASN:HA	1.59	0.44
2:F:130:GLU:OE2	2:F:136:LYS:O	2.35	0.44
2:F:214:LYS:H	2:F:214:LYS:HD2	1.83	0.44
2:F:225:GLN:HE21	2:F:227:ILE:HD11	1.81	0.44
1:A:47:ILE:HD12	1:A:47:ILE:H	1.83	0.44
1:A:118:PRO:HB2	1:A:187:ILE:CG2	2.47	0.44
2:B:124:PHE:CD1	2:B:124:PHE:N	2.86	0.44
3:C:61:LEU:HD12	3:C:61:LEU:N	2.30	0.44
1:E:123:LEU:CD1	2:F:126:PRO:HA	2.47	0.44
3:C:91:THR:O	3:C:91:THR:HG22	2.17	0.44
4:D:160:ARG:HG3	4:D:190:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:PHE:HE2	2:F:174:LYS:O	2.00	0.44
3:G:111:ASP:OD1	3:G:112:ASN:N	2.45	0.44
3:G:142:ARG:C	3:G:144:TYR:H	2.26	0.44
3:G:168:HIS:CG	3:G:169:TRP:N	2.86	0.44
4:H:64:VAL:HG12	4:H:65:ARG:N	2.32	0.44
2:B:36:ASP:OD2	2:B:85:SER:HB2	2.18	0.44
2:B:175:GLU:O	2:B:177:ASN:N	2.51	0.44
1:E:79:SER:HB2	1:E:109:VAL:HG21	2.00	0.44
4:H:184:VAL:O	4:H:185:LEU:HD12	2.18	0.44
1:A:162:ASP:OD2	1:A:169:LYS:NZ	2.46	0.44
2:F:125:GLU:HA	2:F:126:PRO:HD3	1.88	0.44
3:G:37:LEU:N	3:G:37:LEU:HD12	2.33	0.44
4:H:203:GLU:C	4:H:205:PRO:HD3	2.43	0.44
4:H:207:LEU:H	4:H:207:LEU:HD23	1.83	0.44
1:A:6:SER:O	1:A:8:GLN:N	2.51	0.43
1:E:16:GLU:HG2	1:E:17:THR:H	1.83	0.43
1:E:64:PHE:CD1	1:E:75:HIS:HD2	2.36	0.43
2:F:175:GLU:HB3	2:F:179:SER:O	2.17	0.43
3:G:61:LEU:HD12	3:G:61:LEU:N	2.33	0.43
4:H:3:ALA:HA	4:H:108:ASN:OD1	2.17	0.43
3:C:25:PHE:CD1	3:C:33:PHE:CZ	3.06	0.43
4:D:167:VAL:HG23	4:D:168:GLY:H	1.84	0.43
4:H:124:PRO:CD	4:H:205:PRO:HG2	2.47	0.43
3:C:46:LEU:HA	3:C:47:PRO:HD2	1.86	0.43
3:C:88:PRO:HA	3:C:112:ASN:O	2.18	0.43
3:C:165:LYS:HB2	3:C:165:LYS:HE3	1.81	0.43
4:D:165:GLU:OE1	4:D:167:VAL:HG22	2.18	0.43
4:D:197:VAL:HG12	4:D:216:LYS:HA	2.00	0.43
4:H:143:VAL:HG22	4:H:187:MET:HG2	1.99	0.43
1:A:62:THR:OG1	1:A:75:HIS:HB2	2.18	0.43
1:A:118:PRO:HB2	1:A:187:ILE:HG22	2.01	0.43
2:B:53:THR:HG23	2:B:53:THR:O	2.17	0.43
3:C:105:THR:HA	3:C:153:THR:HA	2.01	0.43
2:F:166:VAL:HG12	2:F:167:SER:N	2.32	0.43
3:G:34:TYR:O	3:G:34:TYR:CG	2.71	0.43
1:A:111:PRO:HG3	1:A:160:VAL:CG2	2.49	0.43
2:B:235:ALA:O	2:B:236:ASP:OXT	2.37	0.43
2:F:23:GLN:HB2	2:F:30:MET:HE3	2.00	0.43
2:F:35:GLN:HE21	2:F:88:PHE:HE2	1.66	0.43
4:H:1:PHE:CE2	4:H:115:HIS:CD2	3.07	0.43
4:H:193:ARG:O	4:H:196:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:GLU:HG2	1:E:17:THR:N	2.32	0.43
1:E:111:PRO:O	1:E:112:ASN:C	2.62	0.43
2:F:95:TRP:CE3	2:F:95:TRP:HA	2.53	0.43
3:G:92:VAL:HG12	3:G:93:PHE:N	2.33	0.43
1:A:34:TRP:HB2	1:A:47:ILE:HD12	2.01	0.43
2:B:128:LYS:HE3	2:B:236:ASP:CG	2.43	0.43
4:D:150:TYR:O	4:D:150:TYR:CG	2.70	0.43
1:E:58:ASP:O	1:E:60:ARG:N	2.51	0.43
1:E:125:ASP:C	1:E:127:ARG:H	2.25	0.43
2:F:114:ARG:HG2	2:F:114:ARG:NH1	2.34	0.43
2:F:153:LEU:CD2	2:F:182:LEU:HD21	2.48	0.43
2:F:206:PHE:O	2:F:224:THR:HG23	2.18	0.43
4:D:65:ARG:CG	4:D:66:TYR:N	2.81	0.43
4:D:117:SER:HB2	4:D:118:LEU:H	1.68	0.43
4:D:156:VAL:CG1	4:D:186:VAL:HG21	2.49	0.43
2:B:166:VAL:HG22	2:B:186:LEU:HD13	1.99	0.43
4:D:5:LYS:N	4:D:5:LYS:CD	2.75	0.43
4:D:191:THR:O	3:G:142:ARG:HD3	2.19	0.43
1:E:176:TRP:CE2	2:F:142:LEU:HD11	2.54	0.43
4:H:104:VAL:O	4:H:105:CYS:C	2.62	0.43
2:B:48:TYR:CZ	3:C:62:GLN:HG2	2.53	0.43
2:B:119:PRO:HD3	2:B:206:PHE:CD2	2.54	0.43
3:C:110:VAL:HG21	3:C:120:ILE:HD11	1.98	0.43
1:E:64:PHE:O	1:E:72:PHE:HA	2.19	0.43
2:F:194:HIS:HA	2:F:234:ARG:H	1.84	0.43
3:G:144:TYR:OH	4:H:55:ARG:HD3	2.19	0.43
4:H:114:THR:HG22	4:H:114:THR:O	2.17	0.43
4:D:118:LEU:H	4:D:118:LEU:HD12	1.82	0.42
2:F:174:LYS:HG2	2:F:175:GLU:H	1.84	0.42
3:G:91:THR:HB	3:G:109:PHE:HB3	2.01	0.42
2:B:147:PHE:HE1	2:B:178:TYR:HA	1.84	0.42
1:E:60:ARG:NH1	1:E:60:ARG:CG	2.82	0.42
2:F:193:TRP:CD1	2:F:194:HIS:N	2.88	0.42
1:A:34:TRP:CZ3	1:A:89:CYS:HB3	2.54	0.42
1:A:132:THR:HG22	1:A:182:PHE:CD1	2.54	0.42
3:C:15:GLN:NE2	3:C:116:PRO:HG2	2.34	0.42
3:C:177:LYS:HD2	3:C:177:LYS:HA	1.76	0.42
4:D:73:HIS:HE1	4:D:97:THR:HG21	1.84	0.42
4:D:81:ARG:HB3	4:D:81:ARG:CZ	2.48	0.42
1:A:58:ASP:O	1:A:60:ARG:N	2.51	0.42
3:C:15:GLN:HE22	3:C:115:PRO:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:ASN:HB2	4:D:48:GLN:CB	2.49	0.42
4:D:144:CYS:O	4:D:144:CYS:SG	2.77	0.42
2:F:209:LEU:H	2:F:209:LEU:HG	1.66	0.42
4:H:78:GLU:C	4:H:80:GLY:H	2.27	0.42
3:C:15:GLN:HA	4:D:33:PHE:O	2.19	0.42
2:F:211:GLU:O	2:F:212:GLU:C	2.63	0.42
1:A:57:GLU:O	1:A:58:ASP:C	2.62	0.42
1:A:131:SER:O	1:A:132:THR:C	2.61	0.42
2:B:225:GLN:NE2	2:B:227:ILE:HD11	2.32	0.42
3:G:61:LEU:H	3:G:61:LEU:CD1	2.33	0.42
3:G:99:LEU:HB2	3:G:102:GLN:HB3	2.01	0.42
1:A:53:SER:O	1:A:54:ASN:CB	2.67	0.42
1:A:111:PRO:HG3	1:A:160:VAL:HG21	2.00	0.42
2:B:23:GLN:HB2	2:B:30:MET:HE3	2.01	0.42
2:B:35:GLN:HE21	2:B:88:PHE:HE2	1.68	0.42
3:C:16:SER:HB3	3:C:71:LEU:HD12	2.02	0.42
1:E:161:LEU:HD13	1:E:162:ASP:N	2.34	0.42
2:F:36:ASP:OD2	2:F:85:SER:HB3	2.20	0.42
2:F:153:LEU:HD23	2:F:153:LEU:H	1.85	0.42
3:G:49:PHE:CD2	4:H:116:THR:OG1	2.72	0.42
1:A:97:ASN:OD1	3:C:59:GLY:HA2	2.19	0.42
3:C:22:GLN:HE21	3:C:24:THR:CG2	2.32	0.42
3:C:113:ILE:O	3:C:114:PHE:HB2	2.20	0.42
4:D:189:GLU:OE1	4:D:189:GLU:HA	2.19	0.42
1:E:138:ASP:HA	1:E:170:SER:HB2	2.01	0.42
4:H:31:ARG:O	4:H:31:ARG:HG3	2.20	0.42
4:H:40:GLU:OE2	4:H:55:ARG:NE	2.51	0.42
2:B:80:THR:OG1	2:B:83:GLN:HG3	2.20	0.42
2:B:230:GLU:O	2:B:231:ALA:HB2	2.20	0.42
3:C:66:VAL:HG11	4:D:8:ALA:O	2.19	0.42
4:D:48:GLN:HA	4:D:48:GLN:HE21	1.84	0.42
1:E:132:THR:HB	1:E:182:PHE:CE2	2.55	0.42
2:F:7:ARG:HB3	2:F:7:ARG:HH11	1.84	0.42
1:E:37:GLN:HE22	2:F:35:GLN:HE22	1.68	0.42
3:G:152:LEU:C	3:G:152:LEU:HD22	2.45	0.42
1:A:41:GLU:HB2	1:A:42:SER:H	1.48	0.41
1:A:161:LEU:HB2	2:B:185:ARG:NH1	2.33	0.41
3:C:111:ASP:OD1	3:C:112:ASN:N	2.46	0.41
3:C:142:ARG:O	4:H:193:ARG:HD3	2.20	0.41
4:D:43:PHE:CE2	4:D:109:TYR:HB2	2.55	0.41
1:E:19:ILE:HG22	1:E:75:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:PHE:CG	3:G:33:PHE:CZ	3.07	0.41
3:G:168:HIS:CG	3:G:169:TRP:H	2.38	0.41
4:H:38:MET:HE2	4:H:40:GLU:OE2	2.20	0.41
4:H:113:GLU:C	4:H:118:LEU:HD12	2.45	0.41
4:D:203:GLU:C	4:D:205:PRO:HD3	2.45	0.41
4:D:212:THR:O	4:D:212:THR:HG22	2.16	0.41
1:E:47:ILE:N	1:E:47:ILE:HD12	2.34	0.41
1:E:180:THR:HB	1:E:181:SER:H	1.47	0.41
2:F:84:THR:HG21	2:F:108:THR:HG23	2.02	0.41
1:A:3:VAL:HG12	1:A:4:ARG:N	2.34	0.41
1:A:24:TYR:CD1	1:A:24:TYR:C	2.98	0.41
2:B:62:TYR:CD1	2:B:62:TYR:N	2.88	0.41
1:E:24:TYR:CE2	1:E:32:PHE:CE2	3.09	0.41
2:F:116:VAL:HG13	2:F:148:PRO:HD2	2.01	0.41
4:H:126:VAL:CG2	4:H:202:VAL:HG21	2.51	0.41
2:B:33:TYR:CZ	2:B:43:LEU:HD13	2.55	0.41
2:B:44:ILE:HG22	2:B:45:HIS:ND1	2.36	0.41
3:C:96:SER:HB3	3:C:97:PRO:HD2	2.01	0.41
4:D:63:TYR:HD1	4:D:63:TYR:H	1.68	0.41
4:D:169:VAL:O	4:H:173:GLN:HA	2.21	0.41
3:G:15:GLN:NE2	3:G:115:PRO:HB2	2.35	0.41
2:B:84:THR:CG2	2:B:108:THR:HA	2.46	0.41
4:D:157:ARG:HD2	4:D:164:GLU:OE1	2.20	0.41
1:E:161:LEU:HD23	2:F:167:SER:HB2	2.01	0.41
2:F:69:GLN:CD	2:F:69:GLN:O	2.63	0.41
3:G:44:TRP:O	3:G:45:MET:C	2.63	0.41
4:H:128:ILE:HG22	4:H:129:SER:N	2.36	0.41
3:G:63:ASN:O	3:G:67:VAL:CG2	2.68	0.41
1:A:16:GLU:HG2	1:A:17:THR:H	1.85	0.41
1:A:38:PHE:C	1:A:40:GLY:N	2.78	0.41
1:E:42:SER:HB3	2:F:102:GLY:O	2.19	0.41
2:F:62:TYR:CD1	2:F:62:TYR:N	2.89	0.41
3:G:123:LEU:HB2	3:G:163:ASP:HB2	2.02	0.41
3:G:124:ARG:C	3:G:126:SER:H	2.27	0.41
4:H:207:LEU:HD23	4:H:207:LEU:N	2.35	0.41
2:B:95:TRP:HA	2:B:95:TRP:CE3	2.56	0.41
1:E:34:TRP:CZ3	1:E:89:CYS:HB3	2.56	0.41
2:F:84:THR:HG23	2:F:107:LEU:O	2.21	0.41
2:F:193:TRP:C	2:F:195:ASN:H	2.29	0.41
2:F:215:TRP:HA	2:F:215:TRP:CE3	2.55	0.41
3:G:96:SER:O	3:G:97:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:97:THR:HA	4:H:100:GLU:HG3	2.03	0.41
1:A:79:SER:HB2	1:A:109:VAL:HG21	2.03	0.41
2:B:36:ASP:OD2	2:B:85:SER:HB3	2.20	0.41
2:B:128:LYS:HA	2:B:131:ILE:CD1	2.50	0.41
1:E:60:ARG:HD2	1:E:77:ALA:O	2.20	0.41
1:E:137:THR:O	1:E:138:ASP:HB2	2.19	0.41
2:F:95:TRP:CH2	3:G:62:GLN:CB	3.03	0.41
2:F:128:LYS:HE3	2:F:128:LYS:HB2	1.93	0.41
2:F:128:LYS:O	2:F:131:ILE:HG13	2.21	0.41
4:H:70:VAL:O	4:H:70:VAL:HG12	2.21	0.41
4:H:160:ARG:HG3	4:H:190:MET:CE	2.50	0.41
1:E:114:GLN:C	1:E:116:PRO:HD3	2.46	0.41
1:E:123:LEU:HD23	1:E:133:LEU:O	2.21	0.41
1:E:123:LEU:HB3	2:F:124:PHE:HB3	2.02	0.41
3:G:69:HIS:O	3:G:73:VAL:HG23	2.20	0.41
3:G:135:GLU:OE2	3:G:148:LYS:HD3	2.21	0.41
3:G:140:VAL:HG12	4:H:36:GLN:OE1	2.21	0.41
3:C:2:GLU:HB3	3:C:3:ALA:H	1.69	0.40
3:G:74:LEU:HD11	4:H:63:TYR:CE2	2.56	0.40
4:H:38:MET:CE	4:H:40:GLU:CD	2.94	0.40
4:H:96:ARG:HH11	4:H:96:ARG:CG	2.27	0.40
4:H:123:GLN:H	4:H:123:GLN:HE21	1.69	0.40
1:E:51:PRO:O	1:E:52:VAL:CG2	2.65	0.40
4:H:1:PHE:CE2	4:H:115:HIS:NE2	2.90	0.40
4:H:179:ASP:OD2	4:H:179:ASP:N	2.53	0.40
4:H:192:PRO:HA	4:H:198:TYR:OH	2.21	0.40
1:A:33:PRO:HD2	1:A:90:ALA:O	2.20	0.40
3:C:143:ASP:OD2	3:C:143:ASP:C	2.63	0.40
4:D:59:ASN:HB3	4:D:60:ARG:H	1.63	0.40
1:E:6:SER:O	1:E:8:GLN:N	2.54	0.40
1:E:38:PHE:C	1:E:40:GLY:N	2.80	0.40
1:E:41:GLU:HB2	1:E:42:SER:H	1.49	0.40
1:E:99:ILE:HG22	1:E:100:PHE:N	2.35	0.40
2:B:12:VAL:HG22	2:B:13:THR:N	2.36	0.40
2:B:119:PRO:HG3	2:B:204:VAL:CG1	2.52	0.40
3:C:37:LEU:N	3:C:37:LEU:CD1	2.84	0.40
4:D:160:ARG:HH11	4:D:190:MET:CE	2.34	0.40
1:E:129:GLN:HE21	1:E:129:GLN:HB2	1.68	0.40
4:H:150:TYR:N	4:H:151:PRO:HD3	2.36	0.40
4:H:173:GLN:O	4:H:174:LEU:C	2.64	0.40
3:C:5:HIS:O	4:H:163:GLN:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:GLU:HG2	4:D:73:HIS:N	2.34	0.40
4:D:154:ILE:C	4:D:155:LYS:HD2	2.47	0.40
4:D:199:THR:HG23	4:D:214:GLU:CG	2.41	0.40
4:H:122:GLU:HB3	4:H:149:PHE:HA	2.03	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	183/185 (99%)	135 (74%)	29 (16%)	19 (10%)	0	2
1	E	182/185 (98%)	135 (74%)	30 (16%)	17 (9%)	0	3
2	B	223/236 (94%)	177 (79%)	31 (14%)	15 (7%)	1	6
2	F	234/236 (99%)	189 (81%)	27 (12%)	18 (8%)	1	5
3	C	180/182 (99%)	154 (86%)	19 (11%)	7 (4%)	2	15
3	G	180/182 (99%)	149 (83%)	24 (13%)	7 (4%)	2	15
4	D	186/217 (86%)	151 (81%)	20 (11%)	15 (8%)	1	4
4	H	186/217 (86%)	150 (81%)	25 (13%)	11 (6%)	1	8
All	All	1554/1640 (95%)	1240 (80%)	205 (13%)	109 (7%)	1	6

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	53	SER
1	A	57	GLU
1	A	60	ARG
1	A	128	SER
1	A	180	THR

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Mol	Chain	Res	Type
1	A	181	SER
2	B	126	PRO
2	B	149	ASP
2	B	174	LYS
3	C	3	ALA
3	C	5	HIS
4	D	114	THR
4	D	117	SER
1	E	52	VAL
1	E	53	SER
1	E	57	GLU
1	E	60	ARG
1	E	128	SER
2	F	115	ASP
2	F	209	LEU
3	G	3	ALA
3	G	5	HIS
4	H	190	MET
4	H	206	SER
1	A	59	GLY
1	A	130	ASP
1	A	185	GLN
2	B	5	SER
2	B	96	GLY
2	B	115	ASP
2	B	175	GLU
2	B	179	SER
2	B	209	LEU
3	C	100	LEU
4	D	118	LEU
4	D	154	ILE
4	D	190	MET
4	D	204	HIS
4	D	206	SER
4	D	210	PRO
1	E	14	GLU
1	E	59	GLY
1	E	130	ASP
1	E	180	THR
1	E	181	SER
2	F	5	SER
2	F	85	SER

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Mol	Chain	Res	Type
2	F	96	GLY
2	F	126	PRO
2	F	149	ASP
2	F	211	GLU
2	F	212	GLU
2	F	214	LYS
4	H	105	CYS
4	H	152	ALA
4	H	154	ILE
4	H	210	PRO
1	A	14	GLU
1	A	166	MET
1	A	169	LYS
2	B	85	SER
2	B	176	SER
2	B	224	THR
3	C	2	GLU
3	C	80	SER
4	D	109	TYR
1	E	15	GLY
1	E	132	THR
2	F	176	SER
2	F	216	PRO
3	G	80	SER
3	G	126	SER
4	H	194	ARG
1	A	7	PRO
1	A	133	LEU
2	B	191	THR
2	B	231	ALA
3	C	126	SER
4	D	151	PRO
4	D	173	GLN
1	E	7	PRO
2	F	53	THR
2	F	179	SER
2	F	217	GLU
2	F	233	GLY
4	H	151	PRO
4	H	173	GLN
1	A	15	GLY
1	A	54	ASN

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Mol	Chain	Res	Type
2	B	53	THR
4	D	48	GLN
1	E	54	ASN
1	E	127	ARG
2	F	175	GLU
3	G	10	GLY
3	G	17	PRO
4	H	150	TYR
4	H	204	HIS
1	A	51	PRO
3	C	142	ARG
1	E	51	PRO
1	A	39	PRO
4	D	150	TYR
1	E	39	PRO
3	G	97	PRO
4	D	82	PRO
4	D	205	PRO
2	F	219	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	166/166 (100%)	154 (93%)	12 (7%)	13 39
1	E	165/166 (99%)	153 (93%)	12 (7%)	13 39
2	B	194/202 (96%)	185 (95%)	9 (5%)	24 50
2	F	202/202 (100%)	188 (93%)	14 (7%)	14 40
3	C	163/163 (100%)	156 (96%)	7 (4%)	26 51
3	G	163/163 (100%)	155 (95%)	8 (5%)	22 49
4	D	174/189 (92%)	162 (93%)	12 (7%)	14 40
4	H	174/189 (92%)	157 (90%)	17 (10%)	7 27
All	All	1401/1440 (97%)	1310 (94%)	91 (6%)	15 42

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	33	PRO
1	A	41	GLU
1	A	47	ILE
1	A	56	LYS
1	A	60	ARG
1	A	129	GLN
1	A	133	LEU
1	A	159	THR
1	A	163	MET
1	A	166	MET
1	A	187	ILE
2	B	2	VAL
2	B	31	TYR
2	B	91	SER
2	B	112	ASP
2	B	114	ARG
2	B	149	ASP
2	B	174	LYS
2	B	188	VAL
2	B	223	VAL
3	C	19	ASP
3	C	24	THR
3	C	99	LEU
3	C	127	LYS
3	C	151	TYR
3	C	167	GLU
3	C	172	GLU
4	D	48	GLN
4	D	120	ARG
4	D	121	LEU
4	D	123	GLN
4	D	130	LEU
4	D	169	VAL
4	D	174	LEU
4	D	181	THR
4	D	199	THR
4	D	205	PRO
4	D	210	PRO
4	D	211	ILE
1	E	1	GLN
1	E	33	PRO

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Mol	Chain	Res	Type
1	E	41	GLU
1	E	47	ILE
1	E	56	LYS
1	E	60	ARG
1	E	129	GLN
1	E	133	LEU
1	E	141	SER
1	E	149	MET
1	E	180	THR
1	E	185	GLN
2	F	2	VAL
2	F	31	TYR
2	F	91	SER
2	F	111	GLU
2	F	112	ASP
2	F	115	ASP
2	F	142	LEU
2	F	194	HIS
2	F	213	ASP
2	F	214	LYS
2	F	215	TRP
2	F	223	VAL
2	F	226	ASP
2	F	234	ARG
3	G	4	ASP
3	G	19	ASP
3	G	48	GLU
3	G	62	GLN
3	G	100	LEU
3	G	131	ASP
3	G	152	LEU
3	G	175	VAL
4	H	5	LYS
4	H	44	THR
4	H	48	GLN
4	H	61	GLU
4	H	102	ASP
4	H	118	LEU
4	H	123	GLN
4	H	127	VAL
4	H	155	LYS
4	H	167	VAL

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Mol	Chain	Res	Type
4	H	181	THR
4	H	187	MET
4	H	199	THR
4	H	205	PRO
4	H	206	SER
4	H	210	PRO
4	H	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	75	HIS
1	A	115	ASN
1	A	129	GLN
1	A	142	GLN
1	A	171	ASN
1	A	179	GLN
2	B	4	GLN
2	B	8	ASN
2	B	22	ASN
2	B	23	GLN
2	B	26	ASN
2	B	29	ASN
2	B	35	GLN
2	B	69	GLN
2	B	99	GLN
2	B	133	ASN
2	B	199	HIS
2	B	205	GLN
2	B	225	GLN
3	C	15	GLN
3	C	58	GLN
3	C	62	GLN
3	C	69	HIS
3	C	125	ASN
4	D	48	GLN
4	D	107	HIS
4	D	115	HIS
4	D	123	GLN
4	D	173	GLN
4	D	177	ASN

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Mol	Chain	Res	Type
4	D	183	GLN
1	E	8	GLN
1	E	75	HIS
1	E	115	ASN
1	E	129	GLN
2	F	4	GLN
2	F	22	ASN
2	F	23	GLN
2	F	25	ASN
2	F	26	ASN
2	F	29	ASN
2	F	35	GLN
2	F	69	GLN
2	F	99	GLN
2	F	133	ASN
2	F	135	GLN
2	F	177	ASN
2	F	195	ASN
2	F	205	GLN
2	F	225	GLN
3	G	15	GLN
3	G	58	GLN
3	G	62	GLN
3	G	63	ASN
3	G	85	ASN
3	G	168	HIS
4	H	9	ASN
4	H	48	GLN
4	H	115	HIS
4	H	123	GLN
4	H	173	GLN
4	H	177	ASN
4	H	183	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	185/185 (100%)	-0.10	2 (1%)	78	65	44, 96, 176, 198	0
1	E	184/185 (99%)	-0.24	1 (0%)	87	78	61, 124, 174, 194	0
2	B	227/236 (96%)	-0.26	1 (0%)	88	81	50, 98, 156, 186	0
2	F	236/236 (100%)	-0.36	1 (0%)	88	81	52, 98, 152, 173	0
3	C	182/182 (100%)	-0.42	0	100	100	38, 73, 136, 182	0
3	G	182/182 (100%)	-0.41	1 (0%)	87	78	44, 78, 142, 178	0
4	D	192/217 (88%)	-0.42	0	100	100	43, 77, 122, 152	0
4	H	192/217 (88%)	-0.37	2 (1%)	79	66	45, 85, 127, 168	0
All	All	1580/1640 (96%)	-0.32	8 (0%)	87	78	38, 91, 160, 198	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	3.3
3	G	1	ILE	2.9
1	E	187	ILE	2.5
1	A	187	ILE	2.3
2	F	153	LEU	2.3
4	H	140	ASN	2.1
2	B	222	PRO	2.1
4	H	5	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	E	190	1/1	0.77	0.10	85,85,85,85	0
5	CA	E	189	1/1	0.97	0.04	73,73,73,73	0
5	CA	A	189	1/1	0.97	0.09	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.