Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:54 PM GMT

PDB ID	:	1MLC
Title	:	MONOCLONAL ANTIBODY FAB D44.1 RAISED AGAINST CHICKEN EGG-WHITE LYSOZYME COMPLEXED WITH LYSOZYME
Authors	:	Braden, B.C.; Souchon, H.; Eisele, J.-L.; Bentley, G.A.; Bhat, T.N.; Navaza, J.; Poljak, R.J.
Deposited on	:	1995-03-10
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

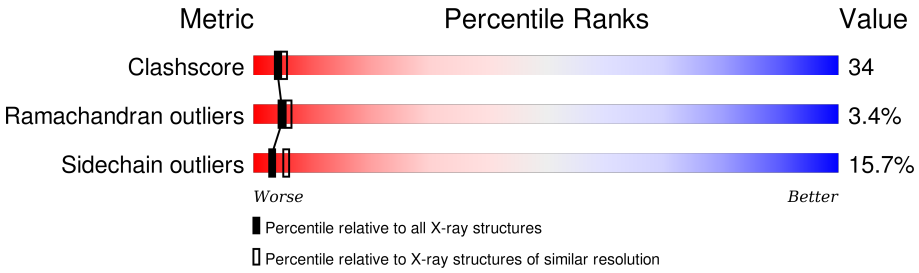
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	42% 42% 15% •
1	C	214	33% 48% 18% •
2	B	218	57% 33% 9% •
2	D	218	45% 45% 8% •
3	E	129	35% 43% 17% 5%
3	F	129	50% 37% 8% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8792 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 IGG1-KAPPA D44.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1658	1023	283	345	7			
1	C	214	Total	C	N	O	S	0	0	0
			1658	1023	283	345	7			

- Molecule 2 is a protein called IGG1-KAPPA D44.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1632	1029	266	329	8			
2	D	218	Total	C	N	O	S	0	0	0
			1632	1029	266	329	8			

- Molecule 3 is a protein called HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
3	F	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	48	Total	O	0	0
			48	48		
4	C	35	Total	O	0	0
			35	35		
4	D	35	Total	O	0	0
			35	35		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	22	Total O 22 22	0	0
4	F	23	Total O 23 23	0	0

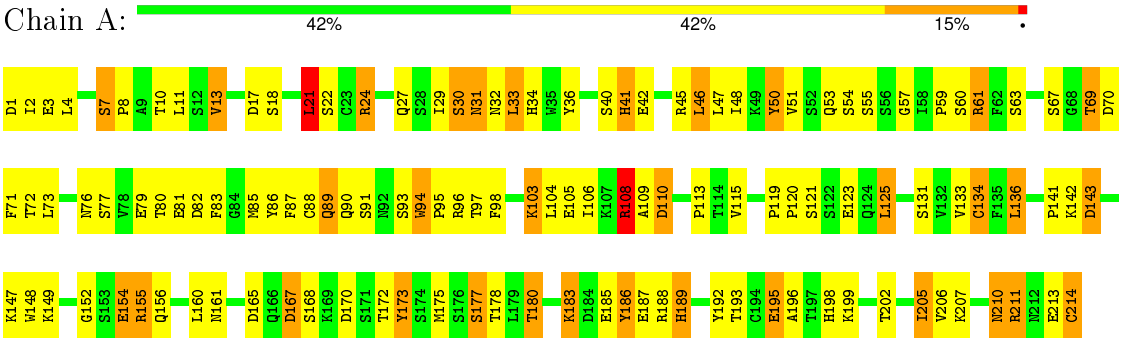
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

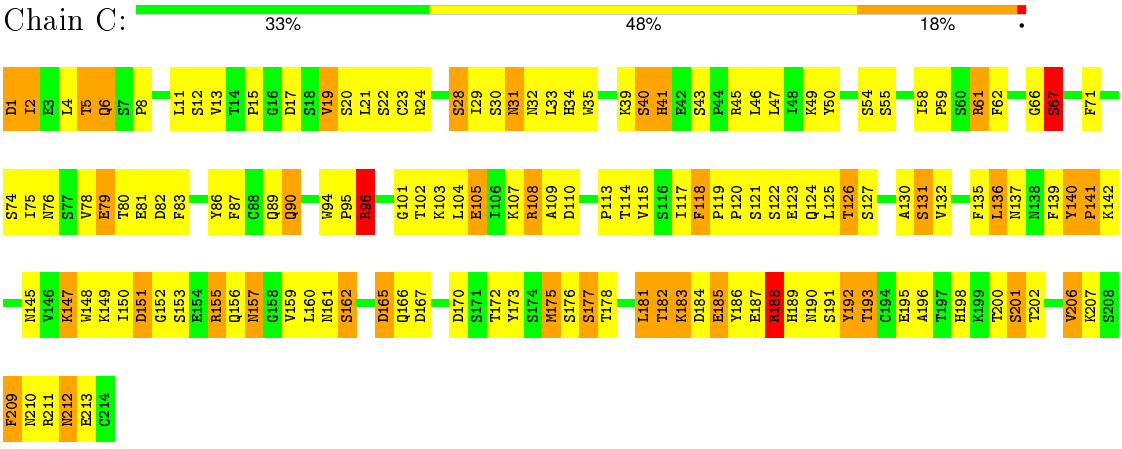
- Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)

Chain A:



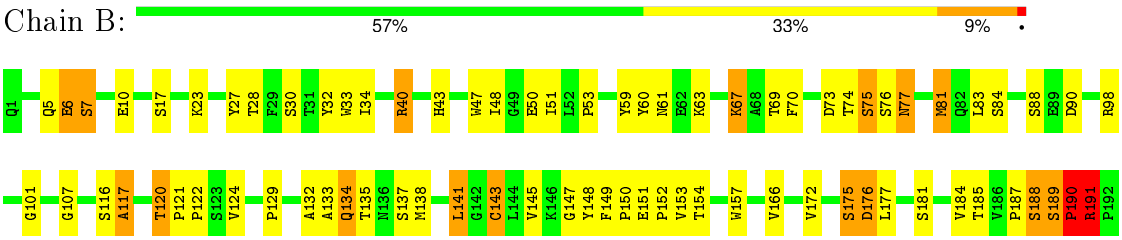
- Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)

Chain C:



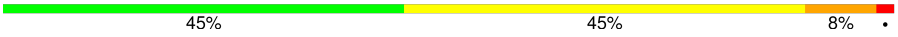
- Molecule 2: IGG1-KAPPA D44.1 FAB (HEAVY CHAIN)

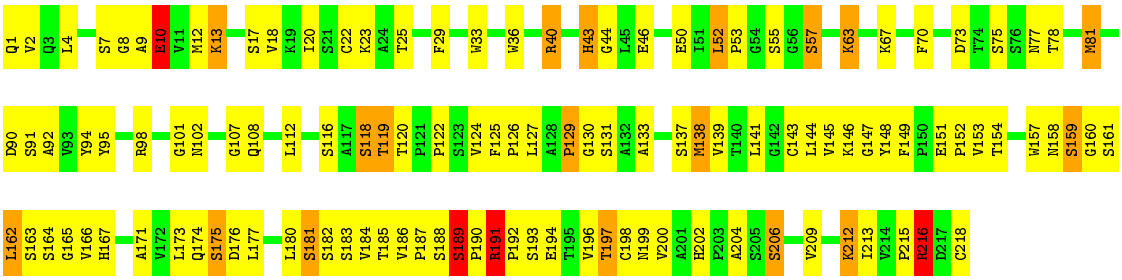
Chain B:



• Molecule 2: IGG1-KAPPA D44.1 FAB (HEAVY CHAIN)

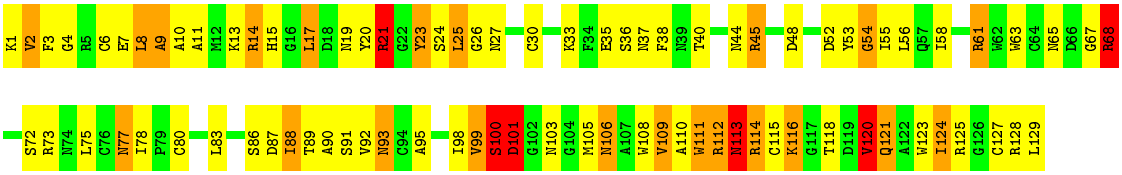
Chain D:





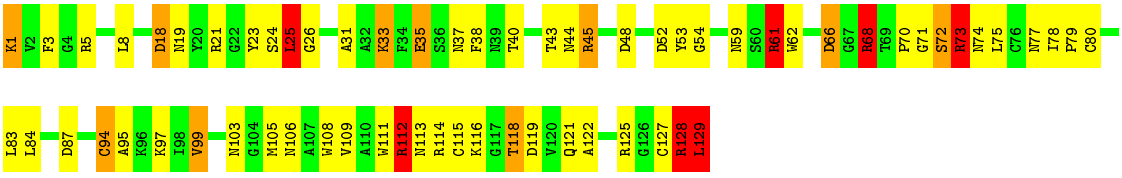
• Molecule 3: HEN EGG WHITE LYSOZYME

Chain E:



• Molecule 3: HEN EGG WHITE LYSOZYME

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.70Å 167.30Å 84.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.00	0/1695	1.93	38/2298 (1.7%)
1	C	0.98	0/1695	1.87	35/2298 (1.5%)
2	B	1.10	1/1676 (0.1%)	1.95	29/2290 (1.3%)
2	D	1.01	1/1676 (0.1%)	1.74	20/2290 (0.9%)
3	E	0.89	0/1021	1.87	25/1379 (1.8%)
3	F	0.97	1/1021 (0.1%)	2.01	29/1379 (2.1%)
All	All	1.00	3/8784 (0.0%)	1.89	176/11934 (1.5%)

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
1	A	0	1
3	E	0	1
3	F	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	101	GLY	N-CA	7.17	1.56	1.46
2	B	101	GLY	N-CA	6.57	1.55	1.46
3	F	35	GLU	CD-OE2	-5.20	1.20	1.25

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	40	ARG	NE-CZ-NH1	20.44	130.52	120.30
3	E	68	ARG	NE-CZ-NH1	19.01	129.80	120.30
1	A	211	ARG	NE-CZ-NH2	-16.75	111.93	120.30
3	E	68	ARG	NE-CZ-NH2	-16.17	112.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	68	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	C	155	ARG	NE-CZ-NH1	14.79	127.69	120.30
2	B	40	ARG	NE-CZ-NH2	-14.36	113.12	120.30
2	B	216	ARG	NE-CZ-NH1	-13.86	113.37	120.30
1	C	17	ASP	CB-CG-OD1	13.53	130.47	118.30
1	C	45	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	A	188	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	C	155	ARG	NE-CZ-NH2	-11.70	114.45	120.30
2	D	40	ARG	NE-CZ-NH2	11.37	125.98	120.30
2	B	216	ARG	NE-CZ-NH2	11.33	125.96	120.30
3	F	73	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	A	108	ARG	NE-CZ-NH1	10.53	125.56	120.30
3	F	68	ARG	NE-CZ-NH2	-10.48	115.06	120.30
3	E	73	ARG	NE-CZ-NH2	10.25	125.42	120.30
3	F	73	ARG	NE-CZ-NH1	9.97	125.29	120.30
2	D	191	ARG	NE-CZ-NH1	9.92	125.26	120.30
2	D	98	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	82	ASP	CB-CG-OD1	-9.67	109.60	118.30
3	F	45	ARG	NE-CZ-NH2	9.65	125.12	120.30
1	C	140	TYR	CB-CG-CD2	9.57	126.74	121.00
3	F	66	ASP	CB-CG-OD1	9.49	126.84	118.30
1	A	211	ARG	NE-CZ-NH1	9.48	125.04	120.30
3	F	61	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	A	108	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	96	ARG	NE-CZ-NH2	9.08	124.84	120.30
2	B	98	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	45	ARG	NE-CZ-NH2	-8.87	115.86	120.30
3	E	68	ARG	CG-CD-NE	8.77	130.22	111.80
1	A	195	GLU	OE1-CD-OE2	8.72	133.76	123.30
3	F	18	ASP	CB-CG-OD2	-8.62	110.55	118.30
2	B	59	TYR	CB-CG-CD1	-8.61	115.83	121.00
1	C	17	ASP	CA-CB-CG	8.46	132.01	113.40
3	F	129	LEU	CA-CB-CG	8.46	134.76	115.30
1	C	140	TYR	CB-CG-CD1	-8.34	116.00	121.00
3	E	48	ASP	CB-CG-OD1	8.30	125.77	118.30
1	C	108	ARG	NE-CZ-NH1	8.27	124.44	120.30
3	F	18	ASP	CB-CG-OD1	8.17	125.65	118.30
2	D	40	ARG	NE-CZ-NH1	-8.14	116.23	120.30
3	E	45	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	B	27	TYR	CB-CG-CD2	-8.01	116.19	121.00
2	B	59	TYR	CB-CG-CD2	8.01	125.80	121.00
1	C	188	ARG	NE-CZ-NH2	-7.94	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	151	GLU	OE1-CD-OE2	7.81	132.67	123.30
3	F	128	ARG	CD-NE-CZ	7.80	134.53	123.60
3	E	61	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	C	108	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	188	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	83	LEU	CA-CB-CG	7.47	132.49	115.30
3	E	128	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	155	ARG	NE-CZ-NH2	7.42	124.01	120.30
3	F	84	LEU	CA-CB-CG	7.41	132.34	115.30
1	A	36	TYR	CB-CG-CD1	-7.37	116.58	121.00
3	F	118	THR	CA-CB-CG2	7.32	122.65	112.40
3	E	23	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	C	17	ASP	CB-CG-OD2	-7.26	111.76	118.30
2	B	176	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	C	192	TYR	CB-CG-CD2	7.16	125.29	121.00
3	E	68	ARG	CD-NE-CZ	7.11	133.56	123.60
1	A	45	ARG	NE-CZ-NH1	7.01	123.81	120.30
3	F	61	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	D	44	GLY	N-CA-C	-6.96	95.71	113.10
3	F	1	LYS	O-C-N	6.95	133.83	122.70
3	F	112	ARG	NE-CZ-NH1	-6.90	116.85	120.30
2	D	40	ARG	CD-NE-CZ	-6.83	114.04	123.60
1	C	110	ASP	CB-CG-OD2	-6.82	112.16	118.30
3	F	112	ARG	CD-NE-CZ	-6.70	114.22	123.60
1	C	54	SER	N-CA-CB	6.64	120.47	110.50
2	D	7	SER	CB-CA-C	6.55	122.55	110.10
1	C	96	ARG	CD-NE-CZ	-6.53	114.46	123.60
3	F	1	LYS	N-CA-CB	6.53	122.35	110.60
1	C	45	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	61	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	C	31	ASN	CB-CA-C	6.47	123.35	110.40
2	B	217	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	33	LEU	CB-CG-CD2	-6.45	100.03	111.00
1	C	79	GLU	OE1-CD-OE2	6.45	131.04	123.30
2	D	73	ASP	O-C-N	6.40	132.94	122.70
1	A	31	ASN	N-CA-CB	-6.39	99.09	110.60
1	A	186	TYR	CB-CG-CD2	6.38	124.83	121.00
1	A	110	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	45	ARG	CD-NE-CZ	-6.37	114.68	123.60
1	C	136	LEU	CB-CA-C	6.35	122.26	110.20
2	D	20	ILE	CA-CB-CG2	6.34	123.59	110.90
2	D	98	ARG	CD-NE-CZ	-6.29	114.80	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	27	TYR	CB-CG-CD1	6.24	124.75	121.00
3	E	17	LEU	CB-CA-C	6.24	122.06	110.20
1	A	36	TYR	CB-CG-CD2	6.24	124.74	121.00
1	C	192	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	17	ASP	CB-CG-OD1	6.20	123.88	118.30
2	D	10	GLU	CB-CA-C	-6.20	98.01	110.40
1	A	103	LYS	N-CA-CB	-6.19	99.45	110.60
1	C	105	GLU	CA-CB-CG	6.18	126.99	113.40
3	E	14	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	B	101	GLY	N-CA-C	-6.12	97.80	113.10
1	A	46	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	165	ASP	CA-CB-CG	6.03	126.67	113.40
3	F	3	PHE	O-C-N	6.00	133.41	123.20
2	B	81	MET	CG-SD-CE	-5.96	90.67	100.20
1	C	181	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	173	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	C	162	SER	O-C-N	5.91	132.15	122.70
3	E	112	ARG	O-C-N	5.87	132.10	122.70
3	F	35	GLU	CG-CD-OE2	5.87	130.04	118.30
1	C	201	SER	C-N-CA	5.86	136.36	121.70
1	C	165	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	165	ASP	CB-CG-OD1	5.84	123.56	118.30
3	F	21	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	61	ARG	CD-NE-CZ	-5.78	115.51	123.60
3	E	21	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	192	TYR	CB-CG-CD1	-5.66	117.60	121.00
3	E	128	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	19	VAL	CA-CB-CG2	5.60	119.30	110.90
3	F	61	ARG	CD-NE-CZ	5.55	131.37	123.60
2	B	120	THR	O-C-N	5.54	131.63	121.10
2	D	63	LYS	CB-CA-C	-5.54	99.33	110.40
2	B	210	ASP	CB-CG-OD2	5.53	123.28	118.30
3	E	54	GLY	C-N-CA	5.53	135.53	121.70
2	D	167	HIS	CA-CB-CG	-5.52	104.21	113.60
3	F	25	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	108	ARG	N-CA-CB	-5.51	100.68	110.60
1	C	209	PHE	O-C-N	5.48	131.47	122.70
3	F	1	LYS	CA-C-O	-5.48	108.60	120.10
3	F	21	ARG	NE-CZ-NH2	-5.45	117.57	120.30
3	E	114	ARG	NE-CZ-NH1	-5.41	117.59	120.30
2	D	46	GLU	OE1-CD-OE2	5.41	129.79	123.30
2	D	189	SER	N-CA-CB	-5.36	102.46	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	23	TYR	CB-CG-CD2	5.36	124.21	121.00
1	C	19	VAL	N-CA-CB	-5.35	99.73	111.50
3	E	111	TRP	C-N-CA	5.34	135.06	121.70
2	B	60	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	D	44	GLY	O-C-N	5.33	131.23	122.70
2	B	6	GLU	CG-CD-OE1	5.32	128.93	118.30
2	D	10	GLU	OE1-CD-OE2	5.32	129.68	123.30
3	F	68	ARG	CD-NE-CZ	5.31	131.03	123.60
1	C	22	SER	N-CA-CB	5.30	118.46	110.50
1	A	21	LEU	CA-CB-CG	5.30	127.49	115.30
3	F	113	ASN	OD1-CG-ND2	5.29	134.06	121.90
1	A	167	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	108	ARG	CA-C-N	-5.27	105.61	117.20
3	F	94	CYS	CB-CA-C	5.26	120.92	110.40
3	E	100	SER	C-N-CA	5.25	134.82	121.70
2	B	7	SER	N-CA-CB	-5.25	102.63	110.50
3	E	73	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	A	69	THR	CA-CB-OG1	-5.23	98.01	109.00
2	B	7	SER	O-C-N	-5.22	114.32	123.20
1	A	189	HIS	CA-CB-CG	-5.21	104.75	113.60
2	B	7	SER	CA-C-N	5.21	126.62	116.20
2	B	197	THR	CA-CB-OG1	-5.20	98.07	109.00
1	A	91	SER	CB-CA-C	5.20	119.98	110.10
3	E	53	TYR	CB-CG-CD2	5.20	124.12	121.00
3	E	73	ARG	CD-NE-CZ	-5.20	116.32	123.60
2	B	83	LEU	CA-C-O	-5.18	109.21	120.10
2	D	198	CYS	O-C-N	5.17	130.97	122.70
1	C	74	SER	O-C-N	5.17	130.97	122.70
2	D	107	GLY	N-CA-C	-5.17	100.18	113.10
2	D	57	SER	O-C-N	5.14	130.93	122.70
1	C	162	SER	N-CA-CB	5.12	118.18	110.50
2	B	195	THR	CA-CB-CG2	5.11	119.56	112.40
3	F	21	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	A	24	ARG	O-C-N	5.10	130.85	122.70
1	A	210	ASN	CA-C-O	-5.09	109.40	120.10
2	B	117	ALA	CB-CA-C	5.09	117.74	110.10
2	B	210	ASP	O-C-N	5.08	130.83	122.70
3	E	75	LEU	CB-CA-C	5.07	119.83	110.20
1	A	50	TYR	C-N-CA	5.06	134.34	121.70
2	B	191	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	94	TRP	CA-C-O	-5.05	109.50	120.10
2	B	197	THR	CA-CB-CG2	5.05	119.47	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	103	ASN	N-CA-C	-5.04	97.38	111.00
1	C	6	GLN	O-C-N	5.04	130.76	122.70
1	A	61	ARG	CA-CB-CG	5.03	124.46	113.40
1	A	96	ARG	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
3	E	68	ARG	Sidechain
3	F	5	ARG	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	1658	0	1572	93	0
1	C	1658	0	1572	165	0
2	B	1632	0	1576	67	0
2	D	1632	0	1576	110	0
3	E	1001	0	959	98	0
3	F	1001	0	959	49	0
4	A	47	0	0	3	0
4	B	48	0	0	3	0
4	C	35	0	0	2	0
4	D	35	0	0	3	0
4	E	22	0	0	0	0
4	F	23	0	0	2	0
All	All	8792	0	8214	560	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 34.

All (560) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLU:HA	1:C:211:ARG:NH1	1.60	1.15
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.29	1.09
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.25	1.08
3:E:121:GLN:HA	3:E:124:ILE:HD11	1.38	1.05
2:D:187:PRO:HD2	2:D:190:PRO:HG2	1.37	1.04
2:D:191:ARG:HH11	2:D:191:ARG:HG3	1.17	1.04
1:C:155:ARG:HG2	1:C:156:GLN:H	1.24	1.03
1:C:11:LEU:HD23	1:C:104:LEU:HD13	1.43	1.00
2:D:10:GLU:HG3	2:D:18:VAL:HG21	1.44	1.00
2:D:70:PHE:CE1	2:D:81:MET:HG3	1.99	0.98
2:D:70:PHE:HE1	2:D:81:MET:HG3	1.24	0.98
3:E:26:GLY:HA3	3:E:120:VAL:HG23	1.46	0.97
2:D:189:SER:HB2	2:D:190:PRO:HD3	1.46	0.97
3:F:62:TRP:CZ3	3:F:73:ARG:HD3	2.02	0.94
1:C:145:ASN:ND2	1:C:147:LYS:HZ3	1.67	0.92
2:B:197:THR:OG1	2:B:212:LYS:HD2	1.72	0.89
1:A:115:VAL:CG1	1:A:207:LYS:HG3	2.03	0.89
1:A:83:PHE:CE2	1:A:106:ILE:HG12	2.08	0.88
1:C:187:GLU:HA	1:C:211:ARG:HH12	1.22	0.88
2:B:48:ILE:HG21	2:B:81:MET:HE1	1.54	0.87
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.56	0.87
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.56	0.87
1:C:124:GLN:HE22	1:C:131:SER:HB2	1.38	0.86
1:C:151:ASP:HA	1:C:191:SER:OG	1.76	0.86
2:D:175:SER:O	2:D:176:ASP:HB2	1.73	0.85
3:E:121:GLN:O	3:E:124:ILE:HG13	1.78	0.83
3:E:121:GLN:HA	3:E:124:ILE:CD1	2.08	0.83
1:C:150:ILE:HG12	1:C:192:TYR:CE1	2.13	0.83
2:D:10:GLU:HG3	2:D:18:VAL:CG2	2.09	0.82
1:A:30:SER:OG	1:A:31:ASN:N	2.08	0.82
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.61	0.82
2:B:187:PRO:HB2	2:B:190:PRO:HD2	1.61	0.82
1:C:155:ARG:HG2	1:C:156:GLN:N	1.93	0.81
2:B:166:VAL:HG22	2:B:184:VAL:HG23	1.61	0.81
3:E:106:ASN:ND2	3:E:111:TRP:HZ3	1.76	0.81
1:A:213:GLU:O	1:A:214:CYS:HB3	1.81	0.80
1:A:80:THR:HA	1:A:83:PHE:CE2	2.17	0.80
3:F:62:TRP:HZ3	3:F:73:ARG:HD3	1.41	0.79
1:A:40:SER:O	1:A:41:HIS:HB2	1.80	0.79
2:D:197:THR:HG23	2:D:212:LYS:HE3	1.64	0.79
1:C:187:GLU:CA	1:C:211:ARG:HH12	1.95	0.79
1:C:150:ILE:HA	1:C:191:SER:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:HA	4:A:1618:HOH:O	1.83	0.78
1:C:66:GLY:O	1:C:67:SER:HB2	1.83	0.78
2:B:48:ILE:HG21	2:B:81:MET:CE	2.12	0.78
1:C:11:LEU:HD23	1:C:104:LEU:CD1	2.13	0.78
1:C:195:GLU:HB2	1:C:206:VAL:HG13	1.64	0.77
3:F:68:ARG:HD2	4:F:2109:HOH:O	1.83	0.77
3:F:121:GLN:HG3	3:F:122:ALA:N	1.99	0.77
2:D:23:LYS:HB3	2:D:23:LYS:NZ	2.00	0.76
3:E:106:ASN:HD22	3:E:111:TRP:HZ3	1.32	0.76
1:A:2:ILE:HD11	1:A:27:GLN:HE21	1.51	0.76
2:D:145:VAL:HG11	2:D:153:VAL:HG21	1.67	0.76
2:D:189:SER:HB2	2:D:190:PRO:CD	2.16	0.76
3:E:21:ARG:HG3	3:E:21:ARG:HH11	1.50	0.75
2:D:138:MET:HG2	2:D:185:THR:HG22	1.69	0.75
3:E:10:ALA:CB	3:E:14:ARG:HH21	2.00	0.74
1:C:166:GLN:HB2	1:C:173:TYR:CE1	2.23	0.74
1:C:181:LEU:HD13	1:C:186:TYR:HA	1.68	0.74
3:F:119:ASP:OD2	3:F:125:ARG:NH2	2.21	0.73
1:C:115:VAL:HG12	1:C:207:LYS:HG3	1.70	0.73
3:E:125:ARG:HA	3:E:125:ARG:HE	1.53	0.73
1:C:8:PRO:HG3	1:C:11:LEU:HD13	1.71	0.73
3:E:106:ASN:HD21	3:E:116:LYS:HE3	1.52	0.72
1:C:90:GLN:HE21	1:C:90:GLN:C	1.92	0.72
1:A:80:THR:HA	1:A:83:PHE:HE2	1.53	0.72
3:E:36:SER:OG	3:E:55:ILE:HA	1.90	0.71
2:D:191:ARG:NH1	2:D:191:ARG:HG3	1.93	0.71
1:A:160:LEU:HD21	2:B:172:VAL:HG23	1.71	0.71
3:E:125:ARG:HA	3:E:125:ARG:NE	2.04	0.71
3:E:21:ARG:CG	3:E:21:ARG:HH11	2.04	0.70
2:D:191:ARG:HH11	2:D:191:ARG:CG	1.97	0.70
3:E:10:ALA:O	3:E:13:LYS:HG2	1.91	0.70
3:F:111:TRP:CZ3	3:F:116:LYS:HE2	2.25	0.70
1:C:11:LEU:HD22	1:C:21:LEU:HD21	1.72	0.70
3:E:98:ILE:O	3:E:101:ASP:HB2	1.92	0.70
1:C:11:LEU:CD2	1:C:21:LEU:HD21	2.22	0.69
2:D:159:SER:O	2:D:161:SER:N	2.26	0.69
2:D:13:LYS:HD2	2:D:116:SER:HA	1.75	0.69
2:D:191:ARG:HD2	2:D:192:PRO:HA	1.74	0.68
1:C:212:ASN:OD1	1:C:212:ASN:N	2.25	0.68
2:D:23:LYS:HZ2	2:D:23:LYS:HB3	1.58	0.68
2:D:129:PRO:HG3	2:D:141:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HD2	2:B:216:ARG:NH2	2.08	0.68
2:D:146:LYS:NZ	2:D:174:GLN:HE21	1.92	0.68
3:E:87:ASP:O	3:E:89:THR:N	2.27	0.68
2:D:161:SER:O	2:D:163:SER:N	2.26	0.68
3:E:17:LEU:HD11	3:E:92:VAL:HG13	1.76	0.68
3:E:116:LYS:O	3:E:118:THR:HG23	1.94	0.67
1:C:11:LEU:HD21	1:C:19:VAL:HG22	1.76	0.67
1:C:136:LEU:C	1:C:137:ASN:HD22	1.98	0.67
2:B:203:PRO:O	2:B:205:SER:N	2.28	0.67
2:D:138:MET:HG3	2:D:186:VAL:C	2.15	0.67
3:E:33:LYS:HG2	3:E:123:TRP:CH2	2.29	0.66
1:C:125:LEU:O	1:C:183:LYS:HD2	1.95	0.66
1:C:108:ARG:NE	1:C:109:ALA:O	2.26	0.66
1:C:150:ILE:O	1:C:151:ASP:C	2.34	0.66
3:E:4:GLY:O	3:E:8:LEU:HB2	1.96	0.66
3:E:108:TRP:O	3:E:111:TRP:N	2.23	0.65
1:A:2:ILE:CD1	1:A:27:GLN:HE21	2.09	0.65
1:C:124:GLN:NE2	1:C:131:SER:HB2	2.10	0.65
1:C:148:TRP:O	1:C:149:LYS:HG3	1.97	0.65
1:C:181:LEU:HD12	1:C:186:TYR:HD1	1.62	0.65
1:C:8:PRO:CG	1:C:11:LEU:HD13	2.27	0.64
1:A:24:ARG:HA	1:A:69:THR:O	1.98	0.64
2:D:191:ARG:CG	2:D:191:ARG:NH1	2.60	0.64
3:E:10:ALA:HB1	3:E:14:ARG:HH21	1.61	0.64
1:A:29:ILE:HD11	1:A:71:PHE:CE1	2.32	0.64
3:E:108:TRP:O	3:E:109:VAL:C	2.35	0.64
3:E:80:CYS:O	3:E:83:LEU:HB2	1.97	0.64
1:A:185:GLU:O	1:A:189:HIS:HD2	1.80	0.64
3:E:26:GLY:CA	3:E:120:VAL:HG23	2.25	0.64
3:F:52:ASP:OD1	3:F:59:ASN:ND2	2.30	0.64
1:C:150:ILE:HG12	1:C:192:TYR:CD1	2.32	0.64
3:E:20:TYR:O	3:E:23:TYR:HB2	1.98	0.63
3:E:56:LEU:HD13	3:E:95:ALA:HB2	1.79	0.63
3:F:61:ARG:NH1	3:F:71:GLY:HA3	2.14	0.63
3:E:27:ASN:ND2	3:E:120:VAL:HG11	2.14	0.63
1:C:47:LEU:HD23	1:C:58:ILE:HD12	1.79	0.63
1:C:145:ASN:HD22	1:C:147:LYS:HZ3	1.45	0.63
2:D:122:PRO:HB3	2:D:148:TYR:HB3	1.81	0.63
2:D:139:VAL:N	2:D:186:VAL:O	2.26	0.62
3:E:52:ASP:HA	3:E:58:ILE:O	1.99	0.62
1:C:184:ASP:OD1	1:C:185:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LYS:O	1:C:186:TYR:HB3	1.99	0.62
1:C:11:LEU:HB3	1:C:104:LEU:HD12	1.81	0.62
2:D:187:PRO:CD	2:D:190:PRO:HG2	2.22	0.62
2:D:192:PRO:HB3	2:D:215:PRO:HG3	1.81	0.62
2:D:52:LEU:HB3	2:D:55:SER:OG	2.00	0.62
1:C:115:VAL:CG1	1:C:207:LYS:HG3	2.29	0.62
1:A:205:ILE:N	1:A:205:ILE:HD12	2.15	0.62
3:E:13:LYS:HD3	3:E:129:LEU:HD22	1.82	0.62
1:C:145:ASN:ND2	1:C:147:LYS:NZ	2.45	0.62
3:E:15:HIS:HB3	3:E:92:VAL:HG11	1.81	0.62
1:A:85:MET:HG2	1:A:87:PHE:CZ	2.34	0.62
3:E:37:ASN:O	3:E:38:PHE:HB2	2.00	0.61
1:C:34:HIS:ND1	2:D:102:ASN:HB3	2.15	0.61
3:E:8:LEU:O	3:E:11:ALA:N	2.33	0.61
3:E:3:PHE:CZ	3:E:88:ILE:HG23	2.35	0.61
1:A:89:GLN:HG2	1:A:90:GLN:N	2.14	0.61
1:A:47:LEU:C	1:A:48:ILE:HG12	2.21	0.61
1:C:166:GLN:HB2	1:C:173:TYR:CZ	2.35	0.61
2:D:138:MET:HA	2:D:187:PRO:HA	1.83	0.61
1:C:2:ILE:HG21	1:C:29:ILE:HG22	1.82	0.61
2:D:180:LEU:HD23	2:D:181:SER:N	2.15	0.61
1:C:150:ILE:HG23	1:C:189:HIS:HB3	1.83	0.61
1:A:149:LYS:HG2	1:A:154:GLU:HA	1.83	0.61
1:C:80:THR:O	1:C:83:PHE:CD2	2.54	0.61
3:E:83:LEU:HD23	3:E:90:ALA:HB1	1.83	0.61
1:C:61:ARG:HH11	1:C:61:ARG:HG3	1.65	0.60
1:C:198:HIS:O	1:C:201:SER:HB2	2.02	0.60
2:D:137:SER:O	2:D:187:PRO:HA	2.01	0.60
1:A:83:PHE:CD2	1:A:106:ILE:CG1	2.84	0.60
2:D:197:THR:CG2	2:D:212:LYS:HE3	2.31	0.60
1:C:188:ARG:HG2	1:C:189:HIS:CE1	2.37	0.60
1:C:71:PHE:HB3	4:C:1813:HOH:O	1.99	0.60
1:A:79:GLU:O	1:A:83:PHE:CE2	2.55	0.60
3:E:30:CYS:O	3:E:33:LYS:HB3	2.02	0.60
1:C:181:LEU:CD1	1:C:186:TYR:HD1	2.15	0.59
1:A:160:LEU:CD2	2:B:172:VAL:HG23	2.32	0.59
3:E:124:ILE:HA	3:E:127:CYS:SG	2.42	0.59
2:B:48:ILE:CD1	2:B:81:MET:HE1	2.32	0.59
1:C:145:ASN:HD22	1:C:147:LYS:NZ	2.01	0.59
2:D:193:SER:HB2	2:D:194:GLU:OE1	2.03	0.59
3:F:121:GLN:CG	3:F:122:ALA:N	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:ALA:O	3:F:35:GLU:HG2	2.03	0.58
1:A:115:VAL:CG1	1:A:207:LYS:CG	2.79	0.58
1:A:119:PRO:HD2	2:B:216:ARG:CZ	2.34	0.58
1:A:115:VAL:HG12	1:A:207:LYS:CG	2.17	0.58
1:C:150:ILE:CD1	1:C:192:TYR:HE1	2.16	0.58
2:D:193:SER:CB	2:D:194:GLU:OE1	2.52	0.58
1:C:59:PRO:HG2	1:C:62:PHE:CE2	2.39	0.58
3:E:13:LYS:CD	3:E:129:LEU:HB3	2.33	0.58
3:F:111:TRP:CH2	3:F:116:LYS:HE2	2.39	0.57
1:A:47:LEU:HD11	1:A:86:TYR:HE2	1.68	0.57
2:D:189:SER:CB	2:D:190:PRO:CD	2.82	0.57
2:D:158:ASN:OD1	2:D:196:VAL:HA	2.04	0.57
3:F:61:ARG:O	3:F:72:SER:HA	2.04	0.57
2:D:187:PRO:C	2:D:190:PRO:HD2	2.25	0.57
2:D:138:MET:HG3	2:D:186:VAL:O	2.05	0.57
1:C:150:ILE:HG21	1:C:189:HIS:CG	2.40	0.57
1:C:29:ILE:HD11	1:C:33:LEU:HD12	1.87	0.57
3:E:20:TYR:O	3:E:23:TYR:CD2	2.58	0.57
1:C:34:HIS:CE1	2:D:102:ASN:HB3	2.39	0.57
3:E:20:TYR:O	3:E:23:TYR:HD2	1.87	0.56
2:D:216:ARG:HA	2:D:216:ARG:CZ	2.35	0.56
1:A:214:CYS:O	1:A:214:CYS:SG	2.63	0.56
1:A:47:LEU:HD11	1:A:86:TYR:CE2	2.40	0.56
1:A:121:SER:O	1:A:125:LEU:HD22	2.05	0.56
3:F:78:ILE:HG13	3:F:79:PRO:HD2	1.86	0.56
1:A:83:PHE:CD2	1:A:106:ILE:HG12	2.40	0.56
2:B:40:ARG:HB3	2:B:43:HIS:HD2	1.71	0.56
1:C:182:THR:OG1	1:C:185:GLU:HB2	2.06	0.56
1:C:29:ILE:HD11	1:C:33:LEU:HB2	1.86	0.56
3:E:9:ALA:HB1	3:E:129:LEU:HD11	1.88	0.56
1:C:124:GLN:HG3	2:D:125:PHE:CE2	2.40	0.55
2:B:40:ARG:HB3	2:B:43:HIS:CD2	2.42	0.55
2:B:10:GLU:HG2	4:B:1708:HOH:O	2.05	0.55
1:C:32:ASN:ND2	3:F:70:PRO:HG3	2.21	0.55
2:D:43:HIS:N	2:D:43:HIS:ND1	2.53	0.55
3:E:113:ASN:HD22	3:E:114:ARG:HG2	1.71	0.55
2:D:90:ASP:O	2:D:94:TYR:OH	2.16	0.55
1:C:182:THR:O	1:C:183:LYS:C	2.44	0.55
2:B:217:ASP:O	2:B:218:CYS:SG	2.65	0.55
3:E:61:ARG:HG3	3:E:61:ARG:NH1	2.20	0.55
2:B:217:ASP:O	2:B:218:CYS:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:ALA:HB3	3:E:14:ARG:HH21	1.70	0.54
3:F:8:LEU:CD2	3:F:38:PHE:HD1	2.20	0.54
2:D:10:GLU:OE1	2:D:10:GLU:HA	2.08	0.54
1:C:29:ILE:HD11	1:C:33:LEU:CD1	2.36	0.54
1:C:32:ASN:HD21	3:F:70:PRO:HG3	1.72	0.54
2:B:147:GLY:HA2	2:B:177:LEU:HB3	1.90	0.54
1:C:28:SER:C	1:C:30:SER:H	2.10	0.54
2:B:209:VAL:HG12	2:B:210:ASP:N	2.22	0.54
3:F:121:GLN:CD	3:F:125:ARG:NH1	2.61	0.54
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.41	0.54
2:D:146:LYS:HZ1	2:D:174:GLN:HE21	1.54	0.54
3:F:94:CYS:O	3:F:97:LYS:N	2.39	0.54
3:E:106:ASN:CG	3:E:112:ARG:HG3	2.29	0.54
3:E:8:LEU:O	3:E:10:ALA:N	2.41	0.53
1:C:66:GLY:O	1:C:67:SER:CB	2.54	0.53
3:E:13:LYS:HD3	3:E:129:LEU:HD13	1.89	0.53
1:A:110:ASP:OD2	1:A:199:LYS:NZ	2.25	0.53
1:C:108:ARG:HH21	1:C:109:ALA:HB3	1.73	0.53
2:D:204:ALA:HB2	4:D:1912:HOH:O	2.09	0.53
1:C:113:PRO:HB3	1:C:139:PHE:CD2	2.44	0.53
1:A:81:GLU:N	1:A:81:GLU:OE1	2.41	0.53
3:E:10:ALA:O	3:E:14:ARG:HG3	2.09	0.53
1:C:124:GLN:O	1:C:127:SER:HB2	2.09	0.53
1:C:15:PRO:HA	1:C:78:VAL:O	2.08	0.53
1:A:29:ILE:O	1:A:32:ASN:HB2	2.09	0.53
1:C:175:MET:HG3	1:C:176:SER:O	2.08	0.53
1:C:125:LEU:HD23	1:C:183:LYS:HG3	1.91	0.53
1:C:147:LYS:HE3	1:C:195:GLU:HG2	1.90	0.53
1:C:21:LEU:HD22	1:C:102:THR:HG21	1.90	0.53
1:A:2:ILE:HG12	1:A:27:GLN:NE2	2.22	0.53
2:D:189:SER:O	2:D:193:SER:OG	2.15	0.53
3:E:89:THR:O	3:E:93:ASN:HB2	2.09	0.53
2:D:129:PRO:HG3	2:D:141:LEU:CD1	2.39	0.52
3:F:8:LEU:HD22	3:F:38:PHE:HD1	1.73	0.52
2:B:203:PRO:C	2:B:205:SER:N	2.62	0.52
2:B:10:GLU:CG	4:B:1708:HOH:O	2.56	0.52
1:A:4:LEU:N	1:A:4:LEU:HD22	2.24	0.52
3:E:1:LYS:HG2	3:E:86:SER:HB3	1.91	0.52
1:C:115:VAL:HA	1:C:135:PHE:O	2.10	0.52
1:C:2:ILE:HG21	1:C:29:ILE:CG2	2.39	0.52
3:F:109:VAL:HG22	3:F:112:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:106:ASN:ND2	3:E:111:TRP:CZ3	2.62	0.52
2:D:157:TRP:O	2:D:162:LEU:HB3	2.10	0.52
1:A:50:TYR:HB2	1:A:53:GLN:HE21	1.74	0.52
2:B:117:ALA:HB2	2:B:176:ASP:HB3	1.91	0.52
1:A:61:ARG:HG3	1:A:76:ASN:O	2.10	0.52
1:A:1:ASP:OD1	1:A:1:ASP:N	2.32	0.52
3:F:23:TYR:CE2	3:F:105:MET:HG3	2.45	0.52
1:C:71:PHE:CD1	1:C:71:PHE:N	2.77	0.51
2:B:147:GLY:O	2:B:177:LEU:HD13	2.10	0.51
2:D:91:SER:O	2:D:92:ALA:HB2	2.08	0.51
3:E:3:PHE:HB2	3:E:8:LEU:HG	1.93	0.51
3:F:111:TRP:CD1	3:F:115:CYS:HB2	2.46	0.51
3:F:103:ASN:O	3:F:106:ASN:HB2	2.10	0.51
1:A:18:SER:OG	3:F:128:ARG:HG3	2.10	0.51
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.41	0.51
1:C:11:LEU:HD21	1:C:19:VAL:CG2	2.41	0.51
2:B:73:ASP:OD1	2:B:75:SER:HB3	2.11	0.51
1:C:181:LEU:HD12	1:C:186:TYR:CD1	2.44	0.51
1:C:150:ILE:CG1	1:C:192:TYR:CE1	2.92	0.51
1:A:205:ILE:H	1:A:205:ILE:HD12	1.76	0.51
2:B:17:SER:HB3	2:B:84:SER:HA	1.93	0.51
1:C:117:ILE:HG22	1:C:207:LYS:HB3	1.93	0.50
1:C:190:ASN:O	1:C:210:ASN:HA	2.11	0.50
1:C:11:LEU:HD22	1:C:21:LEU:CD2	2.40	0.50
3:E:7:GLU:HG2	3:E:7:GLU:O	2.10	0.50
1:C:62:PHE:CD1	1:C:75:ILE:HG12	2.46	0.50
1:A:70:ASP:HB3	4:A:1616:HOH:O	2.10	0.50
2:B:28:THR:HG22	2:B:30:SER:OG	2.11	0.50
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.93	0.50
1:C:79:GLU:O	1:C:82:ASP:HB2	2.11	0.50
3:E:124:ILE:O	3:E:125:ARG:C	2.47	0.50
3:E:27:ASN:HB3	3:E:105:MET:SD	2.52	0.50
2:B:132:ALA:O	2:B:134:GLN:N	2.41	0.50
3:F:62:TRP:HZ3	3:F:73:ARG:CD	2.20	0.50
2:B:150:PRO:HD2	2:B:204:ALA:HB1	1.93	0.50
1:C:122:SER:OG	1:C:123:GLU:OE1	2.28	0.50
3:F:33:LYS:NZ	3:F:37:ASN:OD1	2.30	0.50
3:F:1:LYS:HB3	3:F:40:THR:OG1	2.11	0.50
2:D:187:PRO:O	2:D:190:PRO:HD2	2.12	0.50
1:A:213:GLU:CG	1:A:214:CYS:N	2.72	0.50
2:B:137:SER:HA	2:B:188:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:HA	1:A:205:ILE:O	2.12	0.50
2:D:139:VAL:HG13	2:D:186:VAL:HG22	1.94	0.50
3:E:27:ASN:HD22	3:E:111:TRP:HE1	1.60	0.50
2:D:146:LYS:NZ	2:D:174:GLN:NE2	2.60	0.50
3:E:121:GLN:HA	3:E:124:ILE:CG1	2.42	0.49
1:A:119:PRO:HB2	1:A:120:PRO:HD2	1.93	0.49
3:E:112:ARG:O	3:E:113:ASN:HB2	2.11	0.49
2:B:73:ASP:HB3	2:B:76:SER:OG	2.13	0.49
1:C:40:SER:O	1:C:41:HIS:HB2	2.11	0.49
2:B:187:PRO:HD2	2:B:190:PRO:HG2	1.95	0.49
2:B:150:PRO:HD2	2:B:204:ALA:CB	2.43	0.49
1:A:154:GLU:HG3	1:A:155:ARG:N	2.26	0.49
2:B:203:PRO:C	2:B:205:SER:H	2.15	0.49
1:C:13:VAL:HG21	1:C:104:LEU:HD11	1.95	0.49
1:C:198:HIS:HD2	1:C:200:THR:H	1.60	0.49
1:C:183:LYS:HG2	1:C:187:GLU:OE1	2.12	0.49
1:A:210:ASN:HB2	1:A:213:GLU:HB3	1.94	0.49
2:B:143:CYS:O	2:B:181:SER:HA	2.13	0.49
1:C:125:LEU:CD2	1:C:183:LYS:HG3	2.43	0.49
1:C:162:SER:O	1:C:175:MET:HA	2.12	0.49
3:E:36:SER:OG	3:E:55:ILE:O	2.24	0.48
1:A:141:PRO:HG3	1:A:199:LYS:HD2	1.95	0.48
2:D:202:HIS:CE1	2:D:204:ALA:HB3	2.47	0.48
3:E:110:ALA:O	3:E:114:ARG:HB2	2.12	0.48
3:E:113:ASN:C	3:E:114:ARG:HG2	2.34	0.48
2:B:190:PRO:HD3	4:B:1934:HOH:O	2.12	0.48
1:C:61:ARG:CG	1:C:61:ARG:HH11	2.23	0.48
2:D:50:GLU:OE2	3:F:45:ARG:NH2	2.43	0.48
1:A:161:ASN:HB3	1:A:175:MET:CE	2.43	0.48
3:F:43:THR:HA	3:F:52:ASP:O	2.13	0.48
3:E:61:ARG:O	3:E:72:SER:HA	2.13	0.48
1:C:1:ASP:HB3	4:C:1816:HOH:O	2.13	0.48
1:A:183:LYS:NZ	1:A:187:GLU:OE1	2.47	0.48
1:C:29:ILE:O	1:C:30:SER:HB3	2.13	0.48
2:D:173:LEU:HD23	2:D:177:LEU:O	2.14	0.48
3:F:23:TYR:CD2	3:F:105:MET:HG3	2.48	0.48
1:C:94:TRP:CE3	3:F:45:ARG:HB3	2.48	0.48
2:D:187:PRO:HB2	2:D:190:PRO:HD2	1.94	0.48
1:A:161:ASN:OD1	1:A:177:SER:HB2	2.14	0.48
2:B:150:PRO:O	2:B:202:HIS:NE2	2.44	0.48
2:B:48:ILE:HD12	2:B:81:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:O	1:A:41:HIS:CB	2.56	0.48
2:D:157:TRP:O	2:D:158:ASN:HB2	2.13	0.48
1:C:149:LYS:N	1:C:193:THR:O	2.41	0.48
1:C:8:PRO:HG3	1:C:11:LEU:CD1	2.42	0.48
2:D:10:GLU:HB3	2:D:112:LEU:HD12	1.95	0.48
2:D:192:PRO:CB	2:D:215:PRO:HG3	2.42	0.47
3:E:112:ARG:O	3:E:112:ARG:HD2	2.13	0.47
1:C:170:ASP:OD1	1:C:172:THR:OG1	2.27	0.47
1:C:155:ARG:CG	1:C:156:GLN:N	2.72	0.47
2:D:146:LYS:HZ1	2:D:174:GLN:NE2	2.12	0.47
1:A:83:PHE:CE2	1:A:106:ILE:CG1	2.88	0.47
3:E:21:ARG:CG	3:E:21:ARG:NH1	2.73	0.47
1:C:188:ARG:CG	1:C:189:HIS:CE1	2.96	0.47
1:C:13:VAL:CG2	1:C:104:LEU:HD11	2.45	0.47
3:E:8:LEU:HD12	3:E:38:PHE:CD1	2.49	0.47
2:D:8:GLY:O	2:D:9:ALA:C	2.51	0.47
1:C:137:ASN:HD22	1:C:137:ASN:N	2.10	0.47
2:D:29:PHE:CE2	2:D:53:PRO:HB3	2.50	0.47
2:D:139:VAL:O	2:D:185:THR:HA	2.14	0.47
1:C:33:LEU:HA	1:C:89:GLN:O	2.14	0.47
3:E:99:VAL:O	3:E:101:ASP:N	2.47	0.47
1:C:58:ILE:HA	1:C:59:PRO:HD2	1.81	0.47
1:C:61:ARG:O	1:C:75:ILE:HA	2.15	0.47
2:D:33:TRP:CH2	3:F:45:ARG:NH2	2.81	0.47
3:E:10:ALA:HB3	3:E:14:ARG:NH2	2.30	0.47
2:B:6:GLU:OE2	2:B:107:GLY:HA3	2.14	0.47
2:D:118:SER:O	2:D:119:THR:C	2.51	0.47
1:A:170:ASP:OD1	1:A:172:THR:OG1	2.26	0.47
2:D:139:VAL:HG12	2:D:186:VAL:O	2.14	0.47
1:A:80:THR:HA	1:A:83:PHE:CD2	2.50	0.47
1:A:31:ASN:O	1:A:31:ASN:OD1	2.32	0.47
1:C:142:LYS:HG2	1:C:142:LYS:O	2.14	0.46
2:B:138:MET:HB3	2:B:185:THR:HG22	1.97	0.46
3:E:58:ILE:HG22	3:E:63:TRP:HB2	1.96	0.46
3:F:48:ASP:OD1	3:F:48:ASP:N	2.48	0.46
1:C:86:TYR:O	1:C:101:GLY:HA2	2.15	0.46
1:A:193:THR:HG23	1:A:206:VAL:HG13	1.96	0.46
2:D:153:VAL:CG1	2:D:180:LEU:HD13	2.44	0.46
3:E:13:LYS:HD2	3:E:129:LEU:HB3	1.97	0.46
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.50	0.46
3:F:8:LEU:CD2	3:F:38:PHE:CD1	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD23	1:A:73:LEU:HD23	1.97	0.46
1:A:34:HIS:O	1:A:88:CYS:HA	2.15	0.46
1:C:140:TYR:CD1	1:C:141:PRO:HA	2.51	0.46
2:D:139:VAL:HG22	2:D:141:LEU:CD1	2.46	0.46
3:E:109:VAL:O	3:E:113:ASN:HB3	2.15	0.46
1:A:57:GLY:O	1:A:59:PRO:HD3	2.15	0.46
1:A:11:LEU:HD23	1:A:104:LEU:HD12	1.96	0.46
1:C:39:LYS:HE2	1:C:83:PHE:CE1	2.50	0.46
3:E:25:LEU:HA	3:E:25:LEU:HD22	1.63	0.46
1:C:124:GLN:HE22	1:C:131:SER:CB	2.21	0.46
3:F:80:CYS:O	3:F:83:LEU:HB2	2.16	0.46
3:E:17:LEU:CD1	3:E:92:VAL:HG13	2.44	0.46
2:B:124:VAL:HG21	2:B:200:VAL:HG21	1.98	0.46
2:B:145:VAL:HG11	2:B:153:VAL:HG21	1.98	0.46
1:A:142:LYS:HB2	1:A:173:TYR:CE2	2.51	0.46
1:C:151:ASP:N	1:C:191:SER:O	2.46	0.45
3:E:10:ALA:CB	3:E:14:ARG:NH2	2.76	0.45
1:C:148:TRP:C	1:C:149:LYS:HG3	2.37	0.45
2:D:138:MET:HG2	2:D:185:THR:CG2	2.44	0.45
2:D:91:SER:HA	2:D:112:LEU:O	2.17	0.45
1:C:113:PRO:CB	1:C:139:PHE:HB3	2.36	0.45
3:E:87:ASP:C	3:E:89:THR:H	2.20	0.45
2:B:203:PRO:O	2:B:204:ALA:C	2.53	0.45
2:D:151:GLU:OE2	2:D:171:ALA:HB3	2.17	0.45
1:A:30:SER:HG	1:A:31:ASN:H	1.60	0.45
3:F:121:GLN:OE1	3:F:125:ARG:NH1	2.49	0.45
1:A:21:LEU:O	1:A:72:THR:HA	2.16	0.45
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.29	0.45
1:C:123:GLU:O	1:C:126:THR:OG1	2.28	0.45
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.52	0.45
2:B:48:ILE:HD13	2:B:81:MET:HE1	1.99	0.45
1:C:89:GLN:HG2	1:C:90:GLN:N	2.31	0.45
1:C:167:ASP:HB3	1:C:170:ASP:OD1	2.17	0.45
2:B:47:TRP:O	2:B:61:ASN:ND2	2.46	0.45
1:C:13:VAL:HG21	1:C:19:VAL:HG21	1.97	0.45
2:D:23:LYS:CB	2:D:23:LYS:NZ	2.76	0.45
3:E:8:LEU:HD12	3:E:38:PHE:CE1	2.52	0.45
3:F:114:ARG:HD2	3:F:114:ARG:HH11	1.68	0.45
3:E:111:TRP:HE3	3:E:112:ARG:HB2	1.82	0.45
3:E:3:PHE:CZ	3:E:88:ILE:CG2	3.00	0.45
3:F:99:VAL:HG13	3:F:108:TRP:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLU:C	1:C:189:HIS:H	2.20	0.45
1:C:28:SER:C	1:C:30:SER:N	2.70	0.45
1:C:49:LYS:O	1:C:50:TYR:C	2.56	0.45
1:A:131:SER:OG	1:A:180:THR:HG23	2.17	0.45
1:C:94:TRP:HA	1:C:95:PRO:C	2.37	0.44
3:F:94:CYS:O	3:F:95:ALA:C	2.55	0.44
1:C:170:ASP:C	1:C:170:ASP:OD1	2.56	0.44
1:A:167:ASP:HB3	1:A:170:ASP:OD1	2.17	0.44
1:C:119:PRO:HB3	1:C:209:PHE:CE1	2.52	0.44
3:F:25:LEU:O	3:F:26:GLY:C	2.56	0.44
2:D:139:VAL:HG22	2:D:141:LEU:HD12	1.98	0.44
2:D:52:LEU:O	2:D:53:PRO:C	2.56	0.44
2:D:166:VAL:HG12	2:D:184:VAL:HG23	1.99	0.44
2:B:122:PRO:HB3	2:B:148:TYR:HB3	1.99	0.44
2:D:193:SER:HB3	2:D:194:GLU:OE1	2.17	0.44
2:D:23:LYS:HG3	4:D:1918:HOH:O	2.17	0.44
1:A:119:PRO:HD2	2:B:216:ARG:HH21	1.79	0.44
1:C:61:ARG:HB2	1:C:76:ASN:O	2.17	0.44
2:D:120:THR:HG21	2:D:177:LEU:CD1	2.47	0.44
2:D:148:TYR:O	2:D:149:PHE:HB2	2.18	0.44
1:C:132:VAL:HG12	1:C:148:TRP:CH2	2.52	0.44
1:C:193:THR:HG23	1:C:206:VAL:HG12	1.99	0.44
3:E:113:ASN:O	3:E:114:ARG:HG2	2.18	0.44
1:C:113:PRO:HB3	1:C:139:PHE:CB	2.37	0.44
2:D:180:LEU:HD23	2:D:180:LEU:C	2.38	0.44
3:E:13:LYS:HD3	3:E:129:LEU:HB3	1.98	0.44
1:C:160:LEU:HD11	2:D:174:GLN:OE1	2.16	0.44
1:A:160:LEU:CD2	2:B:172:VAL:CG2	2.95	0.44
1:A:89:GLN:HA	1:A:97:THR:O	2.17	0.44
1:C:39:LYS:HE3	1:C:81:GLU:O	2.17	0.44
2:D:188:SER:O	2:D:191:ARG:O	2.35	0.44
1:A:109:ALA:N	4:A:1627:HOH:O	2.51	0.44
3:E:19:ASN:HD22	3:E:19:ASN:HA	1.35	0.44
2:B:175:SER:O	2:B:176:ASP:HB2	2.18	0.44
1:C:118:PHE:CD2	2:D:127:LEU:CB	3.01	0.44
2:B:197:THR:CG2	2:B:210:ASP:HB3	2.48	0.43
2:B:124:VAL:CG2	2:B:200:VAL:HG21	2.48	0.43
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.58	0.43
2:D:157:TRP:C	2:D:159:SER:N	2.72	0.43
2:B:51:ILE:O	2:B:53:PRO:HD3	2.18	0.43
1:A:143:ASP:O	1:A:198:HIS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:C	1:C:127:SER:H	2.20	0.43
1:C:151:ASP:CA	1:C:191:SER:OG	2.59	0.43
3:E:3:PHE:HE1	3:E:40:THR:CG2	2.31	0.43
1:C:47:LEU:CD2	1:C:58:ILE:HD12	2.46	0.43
3:F:18:ASP:O	3:F:19:ASN:HB2	2.19	0.43
2:D:108:GLN:N	2:D:108:GLN:OE1	2.49	0.43
1:C:96:ARG:HD2	1:C:96:ARG:HH11	1.59	0.43
3:E:77:ASN:C	3:E:77:ASN:OD1	2.56	0.43
2:D:146:LYS:HZ3	2:D:174:GLN:HE21	1.65	0.43
3:E:20:TYR:O	3:E:23:TYR:CB	2.66	0.43
2:D:120:THR:HG21	2:D:177:LEU:HD13	2.00	0.43
3:F:8:LEU:HD22	3:F:38:PHE:CD1	2.52	0.43
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.54	0.43
2:B:50:GLU:OE1	3:E:68:ARG:NH2	2.51	0.43
3:E:27:ASN:ND2	3:E:111:TRP:HE1	2.15	0.43
3:E:95:ALA:HA	3:E:98:ILE:HD12	1.99	0.43
1:C:189:HIS:O	1:C:211:ARG:HD3	2.19	0.43
2:B:132:ALA:O	2:B:133:ALA:HB3	2.19	0.43
1:C:186:TYR:CE1	1:C:192:TYR:CE2	3.06	0.43
1:A:195:GLU:HG2	1:A:206:VAL:CG2	2.22	0.43
1:C:59:PRO:HG2	1:C:62:PHE:CD2	2.54	0.43
1:C:6:GLN:OE1	1:C:87:PHE:HA	2.18	0.43
2:D:36:TRP:HA	2:D:95:TYR:O	2.18	0.43
2:D:40:ARG:HB2	4:D:1929:HOH:O	2.18	0.43
2:B:70:PHE:HE1	2:B:81:MET:CE	2.32	0.43
2:B:33:TRP:CE3	2:B:50:GLU:HG3	2.54	0.43
3:E:8:LEU:C	3:E:10:ALA:N	2.73	0.42
3:E:99:VAL:O	3:E:100:SER:C	2.58	0.42
3:F:35:GLU:OE1	3:F:35:GLU:HA	2.19	0.42
2:D:153:VAL:HG11	2:D:180:LEU:HD13	2.00	0.42
3:E:6:CYS:C	3:E:8:LEU:N	2.73	0.42
2:D:120:THR:O	2:D:148:TYR:HA	2.19	0.42
2:D:2:VAL:HA	2:D:25:THR:O	2.19	0.42
1:C:159:VAL:HA	1:C:178:THR:O	2.20	0.42
1:A:136:LEU:HD21	1:A:196:ALA:HB2	2.00	0.42
1:C:12:SER:HB3	1:C:107:LYS:HB2	2.02	0.42
3:F:62:TRP:O	3:F:75:LEU:HB2	2.20	0.42
1:C:29:ILE:CD1	1:C:33:LEU:HD12	2.48	0.42
1:C:33:LEU:HD13	1:C:71:PHE:CD1	2.54	0.42
2:D:165:GLY:O	2:D:184:VAL:HA	2.19	0.42
1:A:113:PRO:HB2	1:A:136:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:O	1:A:125:LEU:CD2	2.67	0.42
2:B:76:SER:O	2:B:77:ASN:HB2	2.19	0.42
1:A:94:TRP:HA	1:A:95:PRO:C	2.40	0.42
1:C:29:ILE:HG21	1:C:29:ILE:HD13	1.80	0.42
2:D:120:THR:HG22	2:D:147:GLY:O	2.19	0.42
1:A:161:ASN:HB3	1:A:175:MET:HE3	2.00	0.42
1:A:185:GLU:O	1:A:189:HIS:CD2	2.66	0.42
3:E:106:ASN:O	3:E:112:ARG:NE	2.37	0.42
3:E:27:ASN:N	3:E:120:VAL:HG21	2.35	0.42
2:D:147:GLY:O	2:D:177:LEU:HD13	2.19	0.42
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.49	0.42
1:C:150:ILE:HD11	1:C:192:TYR:HE1	1.83	0.41
2:D:40:ARG:HG3	2:D:92:ALA:HB2	2.02	0.41
2:B:189:SER:HB2	2:B:190:PRO:HD3	2.01	0.41
1:C:189:HIS:HB2	1:C:192:TYR:CZ	2.54	0.41
3:E:108:TRP:O	3:E:110:ALA:N	2.52	0.41
2:B:149:PHE:HA	2:B:150:PRO:HA	1.85	0.41
1:C:198:HIS:CD2	1:C:200:THR:H	2.38	0.41
1:C:5:THR:N	1:C:24:ARG:O	2.38	0.41
2:D:124:VAL:HG21	2:D:209:VAL:HB	2.02	0.41
1:C:150:ILE:O	1:C:153:SER:N	2.54	0.41
1:C:188:ARG:O	1:C:188:ARG:HG3	2.20	0.41
1:C:61:ARG:NH1	1:C:61:ARG:CG	2.83	0.41
3:F:127:CYS:HB2	3:F:129:LEU:HD13	2.02	0.41
1:A:2:ILE:CG1	1:A:27:GLN:NE2	2.83	0.41
2:B:191:ARG:HE	2:B:191:ARG:HB3	1.40	0.41
1:C:29:ILE:O	1:C:30:SER:CB	2.67	0.41
2:B:73:ASP:O	2:B:77:ASN:N	2.53	0.41
3:F:40:THR:O	3:F:54:GLY:HA2	2.21	0.41
2:B:214:VAL:HA	2:B:215:PRO:HD3	1.90	0.41
2:B:147:GLY:C	2:B:177:LEU:HD13	2.41	0.41
2:B:50:GLU:CD	3:E:68:ARG:HH22	2.23	0.41
1:C:150:ILE:O	1:C:152:GLY:N	2.54	0.41
2:D:186:VAL:HG23	2:D:187:PRO:O	2.20	0.41
1:C:11:LEU:HD12	1:C:11:LEU:HA	1.82	0.41
1:C:13:VAL:CG2	1:C:19:VAL:HG21	2.51	0.41
1:A:89:GLN:HB2	1:A:98:PHE:CD1	2.56	0.41
2:B:129:PRO:HD3	2:B:141:LEU:HD12	2.02	0.41
1:C:149:LYS:HA	1:C:153:SER:O	2.21	0.41
2:D:10:GLU:HB3	2:D:112:LEU:CD1	2.50	0.41
2:B:157:TRP:HA	2:B:197:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG13	1:A:83:PHE:HE1	1.85	0.41
1:A:94:TRP:CE3	3:E:45:ARG:HB3	2.55	0.41
1:A:186:TYR:CZ	1:A:211:ARG:HD3	2.56	0.41
3:E:8:LEU:O	3:E:9:ALA:C	2.60	0.40
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.79	0.40
1:C:161:ASN:HD22	1:C:177:SER:HA	1.86	0.40
1:A:7:SER:HA	1:A:8:PRO:HA	1.83	0.40
2:D:12:MET:HE3	2:D:12:MET:HB3	1.88	0.40
2:B:120:THR:HA	2:B:121:PRO:HD3	1.80	0.40
1:C:121:SER:HB2	2:D:125:PHE:HB3	2.03	0.40
3:E:121:GLN:C	3:E:124:ILE:HG13	2.41	0.40
1:A:83:PHE:CD2	1:A:106:ILE:HG13	2.55	0.40
1:A:213:GLU:HG3	1:A:214:CYS:N	2.37	0.40
3:F:19:ASN:N	3:F:23:TYR:O	2.54	0.40
3:F:87:ASP:HA	4:F:2112:HOH:O	2.22	0.40
1:C:155:ARG:HD3	1:C:157:ASN:O	2.22	0.40
1:C:198:HIS:HD2	1:C:200:THR:OG1	2.04	0.40
2:D:77:ASN:HD22	2:D:77:ASN:H	1.70	0.40
2:D:138:MET:HA	2:D:186:VAL:O	2.22	0.40
2:D:213:ILE:O	2:D:215:PRO:HD3	2.22	0.40
2:D:23:LYS:HG2	2:D:78:THR:OG1	2.21	0.40
3:E:1:LYS:HD2	3:E:2:VAL:N	2.37	0.40
2:D:154:THR:O	2:D:200:VAL:HA	2.21	0.40
1:C:124:GLN:OE1	1:C:130:ALA:HA	2.22	0.40
3:F:53:TYR:OH	3:F:66:ASP:OD2	2.34	0.40
2:B:32:TYR:CE1	3:E:67:GLY:HA3	2.57	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	212/214 (99%)	199 (94%)	7 (3%)	6 (3%)	6 9
1	C	212/214 (99%)	180 (85%)	26 (12%)	6 (3%)	6 9
2	B	216/218 (99%)	194 (90%)	19 (9%)	3 (1%)	14 24
2	D	216/218 (99%)	175 (81%)	30 (14%)	11 (5%)	2 2
3	E	127/129 (98%)	99 (78%)	18 (14%)	10 (8%)	1 1
3	F	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	12 21
All	All	1110/1122 (99%)	958 (86%)	114 (10%)	38 (3%)	5 6

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
2	B	134	GLN
1	C	67	SER
1	C	213	GLU
2	D	160	GLY
2	D	162	LEU
2	D	164	SER
3	E	88	ILE
3	E	100	SER
3	E	113	ASN
3	F	118	THR
1	A	51	VAL
1	A	60	SER
1	A	67	SER
2	B	190	PRO
2	B	204	ALA
1	C	151	ASP
2	D	130	GLY
2	D	159	SER
2	D	216	ARG
3	E	9	ALA
3	E	109	VAL
1	C	120	PRO
2	D	129	PRO
2	D	131	SER
2	D	133	ALA
2	D	206	SER
3	F	77	ASN
1	A	77	SER
1	C	28	SER

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Mol	Chain	Res	Type
3	E	54	GLY
3	E	77	ASN
3	E	101	ASP
3	E	120	VAL
1	C	193	THR
3	E	35	GLU
1	A	152	GLY
2	D	126	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/194 (100%)	163 (84%)	31 (16%)	3 5
1	C	194/194 (100%)	160 (82%)	34 (18%)	2 4
2	B	184/184 (100%)	159 (86%)	25 (14%)	5 8
2	D	184/184 (100%)	155 (84%)	29 (16%)	3 5
3	E	105/105 (100%)	85 (81%)	20 (19%)	2 3
3	F	105/105 (100%)	92 (88%)	13 (12%)	6 11
All	All	966/966 (100%)	814 (84%)	152 (16%)	3 5

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	SER
1	A	10	THR
1	A	13	VAL
1	A	21	LEU
1	A	22	SER
1	A	30	SER
1	A	42	GLU
1	A	46	LEU
1	A	55	SER

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Mol	Chain	Res	Type
1	A	63	SER
1	A	89	GLN
1	A	93	SER
1	A	103	LYS
1	A	105	GLU
1	A	108	ARG
1	A	123	GLU
1	A	125	LEU
1	A	134	CYS
1	A	136	LEU
1	A	143	ASP
1	A	147	LYS
1	A	154	GLU
1	A	156	GLN
1	A	168	SER
1	A	177	SER
1	A	180	THR
1	A	183	LYS
1	A	202	THR
1	A	205	ILE
1	A	214	CYS
2	B	5	GLN
2	B	7	SER
2	B	23	LYS
2	B	34	ILE
2	B	63	LYS
2	B	67	LYS
2	B	69	THR
2	B	74	THR
2	B	75	SER
2	B	77	ASN
2	B	88	SER
2	B	116	SER
2	B	135	THR
2	B	141	LEU
2	B	143	CYS
2	B	152	PRO
2	B	154	THR
2	B	175	SER
2	B	188	SER
2	B	189	SER
2	B	190	PRO

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Mol	Chain	Res	Type
2	B	191	ARG
2	B	193	SER
2	B	198	CYS
2	B	217	ASP
1	C	1	ASP
1	C	2	ILE
1	C	4	LEU
1	C	5	THR
1	C	20	SER
1	C	31	ASN
1	C	40	SER
1	C	41	HIS
1	C	43	SER
1	C	46	LEU
1	C	55	SER
1	C	61	ARG
1	C	67	SER
1	C	90	GLN
1	C	96	ARG
1	C	103	LYS
1	C	105	GLU
1	C	114	THR
1	C	118	PHE
1	C	126	THR
1	C	131	SER
1	C	141	PRO
1	C	147	LYS
1	C	157	ASN
1	C	165	ASP
1	C	175	MET
1	C	177	SER
1	C	182	THR
1	C	183	LYS
1	C	185	GLU
1	C	188	ARG
1	C	202	THR
1	C	206	VAL
1	C	212	ASN
2	D	1	GLN
2	D	10	GLU
2	D	13	LYS
2	D	17	SER

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Mol	Chain	Res	Type
2	D	43	HIS
2	D	52	LEU
2	D	57	SER
2	D	63	LYS
2	D	67	LYS
2	D	75	SER
2	D	81	MET
2	D	118	SER
2	D	119	THR
2	D	138	MET
2	D	143	CYS
2	D	144	LEU
2	D	152	PRO
2	D	175	SER
2	D	181	SER
2	D	182	SER
2	D	183	SER
2	D	189	SER
2	D	191	ARG
2	D	197	THR
2	D	199	ASN
2	D	206	SER
2	D	212	LYS
2	D	216	ARG
2	D	218	CYS
3	E	2	VAL
3	E	8	LEU
3	E	21	ARG
3	E	24	SER
3	E	25	LEU
3	E	44	ASN
3	E	65	ASN
3	E	68	ARG
3	E	78	ILE
3	E	91	SER
3	E	93	ASN
3	E	99	VAL
3	E	101	ASP
3	E	106	ASN
3	E	113	ASN
3	E	115	CYS
3	E	116	LYS

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Mol	Chain	Res	Type
3	E	120	VAL
3	E	121	GLN
3	E	124	ILE
3	F	24	SER
3	F	25	LEU
3	F	33	LYS
3	F	44	ASN
3	F	61	ARG
3	F	68	ARG
3	F	72	SER
3	F	73	ARG
3	F	74	ASN
3	F	99	VAL
3	F	112	ARG
3	F	128	ARG
3	F	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	32	ASN
1	A	53	GLN
1	A	145	ASN
1	A	189	HIS
1	A	210	ASN
2	B	43	HIS
2	B	134	GLN
2	B	174	GLN
1	C	32	ASN
1	C	53	GLN
1	C	76	ASN
1	C	92	ASN
1	C	137	ASN
1	C	145	ASN
1	C	157	ASN
1	C	161	ASN
1	C	198	HIS
1	C	210	ASN
2	D	77	ASN
2	D	174	GLN
3	E	19	ASN

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Mol	Chain	Res	Type
3	E	27	ASN
3	E	44	ASN
3	E	46	ASN
3	E	106	ASN
3	E	113	ASN
3	F	74	ASN
3	F	93	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.