



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 1DM4 / pdb_00001dm4
Title : SER195ALA MUTANT OF HUMAN THROMBIN COMPLEXED WITH
FIBRINOPEPTIDE A (7-16)
Authors : Krishnan, R.; Sadler, E.J.; Tulinsky, A.
Deposited on : 1999-12-13
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

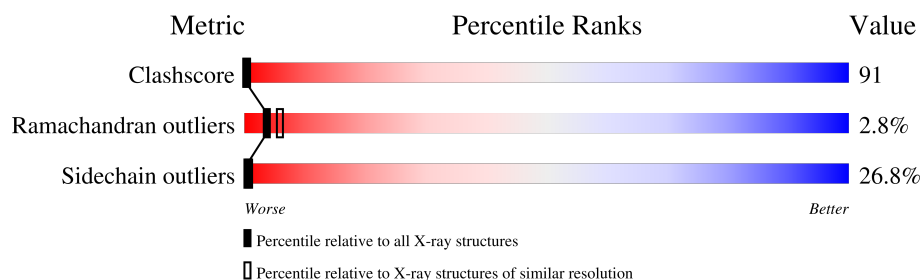
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	35	14% 34% 40% 6% 6%
2	B	260	17% 43% 30% 8% .
3	C	11	9% 45% 36% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2525 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 PROTEIN (ALPHA THROMBIN:LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	33	Total	C	N	O	S	0	0	0
			263	165	42	55	1			

- Molecule 2 is a protein called PROTEIN (MUTANT ALPHA THROMBIN:HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			2038	1299	360	365	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 3 is a protein called PROTEIN (FIBRINOPEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			75	46	13	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	127	Total	O	0	0
			127	127		
4	C	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

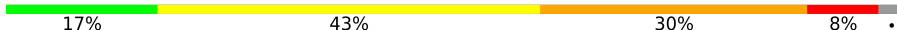
Note EDS was not executed.

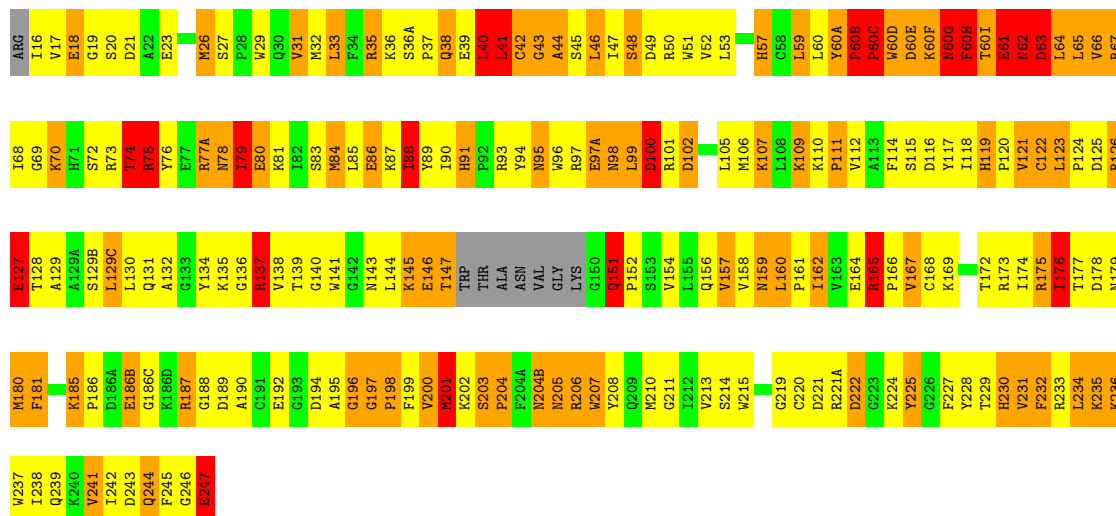
• Molecule 1: PROTEIN (ALPHA THROMBIN:LIGHT CHAIN)

Chain A: 



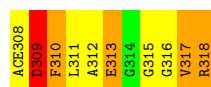
• Molecule 2: PROTEIN (MUTANT ALPHA THROMBIN:HEAVY CHAIN)

Chain B: 



• Molecule 3: PROTEIN (FIBRINOPEPTIDE)

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	135.10Å 135.10Å 135.10Å 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}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.15	0/266	2.25	10/354 (2.8%)
2	B	1.27	3/2090 (0.1%)	2.41	128/2822 (4.5%)
3	C	1.15	0/73	2.54	6/95 (6.3%)
All	All	1.25	3/2429 (0.1%)	2.40	144/3271 (4.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	THR	CA-CB	5.96	1.63	1.53
2	B	77(A)	ARG	C-O	5.51	1.30	1.24
2	B	97(A)	GLU	CA-C	-5.17	1.48	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	ARG	CD-NE-CZ	19.46	151.65	124.40
2	B	21	ASP	CA-CB-CG	12.46	125.06	112.60
3	C	309	ASP	CA-CB-CG	-11.36	101.24	112.60
2	B	165	ARG	CD-NE-CZ	10.90	139.66	124.40
1	A	14(K)	ILE	CA-C-O	10.75	139.08	120.80
2	B	60(H)	PHE	CA-CB-CG	10.40	124.20	113.80
2	B	97(A)	GLU	N-CA-C	10.34	126.30	112.13
2	B	206	ARG	CD-NE-CZ	10.04	138.45	124.40
1	A	1(G)	PHE	CA-CB-CG	-9.95	103.85	113.80
2	B	41	LEU	CB-CA-C	9.80	125.49	109.02
2	B	181	PHE	CA-CB-CG	9.58	123.38	113.80
2	B	119	HIS	CA-C-O	-9.54	111.92	120.13
2	B	44	ALA	CA-C-O	-9.06	111.38	121.25
2	B	204(B)	ASN	OD1-CG-ND2	8.87	131.47	122.60
2	B	119	HIS	O-C-N	8.54	131.13	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	ASN	CA-CB-CG	-8.41	104.19	112.60
2	B	62	ASN	CA-CB-CG	-8.30	104.30	112.60
2	B	62	ASN	OD1-CG-ND2	8.18	130.78	122.60
2	B	127	GLU	CB-CG-CD	8.16	126.48	112.60
2	B	63	ASP	CA-CB-CG	7.98	120.58	112.60
2	B	232	PHE	CA-CB-CG	-7.92	105.88	113.80
2	B	204(B)	ASN	CA-C-N	-7.92	111.36	123.47
2	B	204(B)	ASN	C-N-CA	-7.92	111.36	123.47
2	B	95	ASN	CA-C-O	-7.87	112.04	120.46
2	B	31	VAL	CA-C-O	-7.86	111.76	120.72
2	B	100	ASP	CB-CA-C	7.75	122.28	109.89
2	B	225	TYR	N-CA-C	7.67	121.40	108.90
2	B	205	ASN	N-CA-CB	-7.66	100.31	112.63
2	B	200	VAL	O-C-N	7.63	130.70	122.76
2	B	119	HIS	CA-CB-CG	7.54	121.34	113.80
2	B	129(C)	LEU	CA-C-O	-7.52	111.90	120.24
2	B	206	ARG	NE-CZ-NH2	7.50	125.95	119.20
2	B	137	ARG	CD-NE-CZ	-7.50	113.91	124.40
2	B	151	GLN	CA-C-O	-7.30	113.11	120.63
2	B	19	GLY	CA-C-O	-7.17	114.33	121.93
2	B	70	LYS	N-CA-C	7.15	121.10	110.52
2	B	181	PHE	CA-C-O	-7.13	113.63	121.33
1	A	1(D)	GLY	C-N-CA	7.13	139.53	121.70
2	B	231	VAL	O-C-N	7.08	128.74	121.87
2	B	79	ILE	CA-C-O	-7.01	113.21	120.71
2	B	76	TYR	N-CA-CB	7.00	121.35	110.21
2	B	52	VAL	CB-CA-C	6.95	121.21	110.50
2	B	80	GLU	CA-CB-CG	6.92	127.95	114.10
2	B	204	PRO	N-CA-C	-6.92	105.70	114.35
3	C	313	GLU	CA-C-O	6.87	127.74	119.43
2	B	60(B)	PRO	N-CA-C	6.83	119.03	110.70
2	B	40	LEU	CA-C-N	-6.83	111.52	122.24
2	B	40	LEU	C-N-CA	-6.83	111.52	122.24
1	A	11	SER	CA-C-N	6.80	133.27	122.59
1	A	11	SER	C-N-CA	6.80	133.27	122.59
2	B	67	ARG	CB-CG-CD	6.80	126.94	111.30
2	B	109	LYS	N-CA-C	-6.72	103.98	111.71
1	A	1(C)	GLU	N-CA-C	6.67	125.00	110.80
2	B	123	LEU	N-CA-C	-6.65	101.13	110.31
2	B	91	HIS	CA-CB-CG	-6.63	107.17	113.80
1	A	1(G)	PHE	C-N-CA	6.59	136.14	122.30
2	B	64	LEU	N-CA-C	6.57	120.24	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	PRO	O-C-N	6.57	130.98	123.10
2	B	40	LEU	CA-C-O	-6.56	113.13	120.54
2	B	151	GLN	N-CA-C	-6.55	101.88	110.39
1	A	4	ARG	CD-NE-CZ	6.54	133.56	124.40
2	B	74	THR	N-CA-CB	-6.52	99.48	110.49
2	B	243	ASP	CB-CA-C	6.49	119.21	111.22
2	B	123	LEU	CA-C-O	-6.43	114.21	120.19
2	B	66	VAL	CA-C-O	-6.38	113.45	120.72
2	B	159	ASN	CA-CB-CG	6.32	118.92	112.60
2	B	230	HIS	O-C-N	6.29	131.00	122.57
2	B	151	GLN	CA-CB-CG	-6.28	101.53	114.10
2	B	79	ILE	N-CA-C	6.27	117.84	111.00
2	B	67	ARG	NE-CZ-NH2	6.22	124.79	119.20
2	B	74	THR	N-CA-C	6.19	123.99	110.80
2	B	75	ARG	CD-NE-CZ	6.18	133.06	124.40
2	B	20	SER	CA-C-O	-6.18	114.59	121.51
2	B	179	ASN	CA-C-O	-6.18	112.43	119.78
2	B	160	LEU	CA-C-O	-6.13	114.86	120.50
1	A	1(G)	PHE	CA-C-O	6.12	129.26	120.51
2	B	185	LYS	N-CA-CB	6.11	116.83	109.74
2	B	43	GLY	CA-C-O	-6.05	115.09	121.57
2	B	179	ASN	CA-CB-CG	-6.04	106.56	112.60
2	B	102	ASP	O-C-N	5.99	130.22	122.43
2	B	189	ASP	CA-C-O	-5.96	114.90	121.28
2	B	78	ASN	CB-CA-C	5.96	120.73	110.01
2	B	207	TRP	N-CA-CB	5.93	119.83	110.23
2	B	122	CYS	CA-CB-SG	5.89	127.96	114.40
2	B	73	ARG	N-CA-C	-5.89	105.59	112.89
2	B	203	SER	CA-CB-OG	-5.88	99.33	111.10
2	B	190	ALA	CA-C-O	-5.87	114.32	121.36
2	B	77(A)	ARG	CA-C-N	-5.86	111.77	122.38
2	B	77(A)	ARG	C-N-CA	-5.86	111.77	122.38
2	B	100	ASP	CA-C-O	5.85	127.53	120.81
3	C	310	PHE	N-CA-C	-5.83	104.61	110.97
2	B	98	ASN	CB-CA-C	5.83	118.09	109.29
2	B	196	GLY	O-C-N	5.82	130.26	122.70
2	B	84	MET	CA-C-O	-5.81	114.53	121.56
2	B	75	ARG	CA-CB-CG	5.77	125.63	114.10
2	B	186(B)	GLU	N-CA-C	5.76	120.30	113.28
2	B	35	ARG	NE-CZ-NH2	-5.75	114.02	119.20
2	B	206	ARG	NH1-CZ-NH2	-5.75	111.82	119.30
2	B	18	GLU	CG-CD-OE2	-5.73	105.22	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	121	VAL	CA-C-O	-5.67	115.12	121.98
2	B	146	GLU	CB-CG-CD	5.67	122.23	112.60
2	B	204	PRO	CA-C-O	5.65	125.87	118.98
2	B	157	VAL	CA-C-O	-5.64	114.35	120.67
2	B	165	ARG	NE-CZ-NH2	-5.63	114.14	119.20
2	B	26	MET	CA-C-O	-5.62	113.17	119.79
2	B	79	ILE	CA-CB-CG2	5.56	119.96	110.50
2	B	62	ASN	N-CA-C	5.55	120.05	113.12
2	B	52	VAL	N-CA-CB	-5.53	102.37	111.44
2	B	74	THR	CA-CB-OG1	-5.53	101.31	109.60
2	B	42	CYS	CA-C-N	5.51	126.45	121.82
2	B	42	CYS	C-N-CA	5.51	126.45	121.82
2	B	204(B)	ASN	CB-CG-ND2	-5.51	108.14	116.40
2	B	74	THR	OG1-CB-CG2	5.47	120.25	109.30
2	B	176	ILE	N-CA-CB	-5.46	102.22	111.23
2	B	201	MET	CA-CB-CG	5.45	124.99	114.10
2	B	40	LEU	O-C-N	5.43	129.42	123.22
2	B	73	ARG	CD-NE-CZ	5.40	131.96	124.40
2	B	180	MET	CA-C-O	-5.40	115.46	121.51
2	B	123	LEU	CB-CA-C	5.34	116.11	108.68
2	B	159	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	14(H)	GLU	CG-CD-OE2	-5.33	106.15	118.40
2	B	102	ASP	CA-C-O	-5.33	115.62	121.58
2	B	126	ARG	CA-C-N	5.32	127.41	120.28
2	B	126	ARG	C-N-CA	5.32	127.41	120.28
2	B	20	SER	O-C-N	5.32	129.66	122.96
2	B	42	CYS	CA-CB-SG	5.31	126.62	114.40
2	B	214	SER	N-CA-C	5.27	119.03	111.02
2	B	88	ILE	CA-C-O	-5.27	114.51	120.67
2	B	75	ARG	NE-CZ-NH1	5.26	126.76	121.50
2	B	197	GLY	O-C-N	5.24	127.01	121.77
2	B	73	ARG	O-C-N	5.17	129.59	122.46
2	B	247	GLU	CA-CB-CG	5.15	124.40	114.10
2	B	190	ALA	N-CA-C	-5.14	102.15	110.32
2	B	222	ASP	CA-C-O	-5.13	115.50	121.15
2	B	244	GLN	CB-CG-CD	5.12	121.30	112.60
2	B	235	LYS	N-CA-C	5.09	116.91	111.36
2	B	198	PRO	CB-CA-C	-5.07	103.19	111.56
2	B	160	LEU	O-C-N	5.05	124.94	121.71
2	B	111	PRO	CA-C-O	-5.04	115.26	121.31
2	B	186(C)	GLY	C-N-CA	5.04	134.31	121.70
3	C	318	ARG	CD-NE-CZ	5.03	131.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	TYR	CA-C-O	-5.02	115.21	120.58
3	C	313	GLU	CA-C-N	5.01	128.76	122.00
3	C	313	GLU	C-N-CA	5.01	128.76	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	263	0	258	106	0
2	B	2038	0	2010	351	0
3	C	75	0	69	25	0
4	A	15	0	0	8	0
4	B	127	0	0	51	0
4	C	7	0	0	0	0
All	All	2525	0	2337	427	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 91.

All (427) 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:A:1(F):GLY:HA2	2:B:235:LYS:CE	1.54	1.35
1:A:1(F):GLY:HA2	2:B:235:LYS:NZ	1.46	1.28
1:A:1(G):PHE:CD1	1:A:1(F):GLY:N	2.12	1.17
2:B:89:TYR:HE2	4:B:433:HOH:O	1.29	1.16
1:A:1(C):GLU:HB2	1:A:1(CYS:HB3	1.28	1.10
1:A:1(G):PHE:HD1	1:A:1(F):GLY:CA	1.65	1.09
1:A:1(H):THR:HG22	1:A:1(G):PHE:N	1.67	1.05
2:B:173:ARG:HD3	3:C:313:GLU:OE2	1.57	1.03
1:A:10:LYS:HG3	1:A:12:LEU:CD1	1.90	1.01
1:A:1(G):PHE:HD1	1:A:1(F):GLY:N	1.51	1.01
2:B:201:MET:CE	2:B:210:MET:HG3	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:HD2	2:B:89:TYR:CE2	1.97	1.00
1:A:10:LYS:HG3	1:A:12:LEU:HD11	1.41	0.99
2:B:18:GLU:HB2	2:B:188:GLY:HA2	1.43	0.99
2:B:78:ASN:HB2	4:B:601:HOH:O	1.59	0.99
2:B:126:ARG:HB3	2:B:127:GLU:OE1	1.62	0.97
2:B:85:LEU:HD11	2:B:106:MET:HE3	1.44	0.97
1:A:1(F):GLY:CA	2:B:235:LYS:CE	2.42	0.97
2:B:50:ARG:HD3	4:B:607:HOH:O	1.64	0.97
2:B:57:HIS:NE2	3:C:318:ARG:OXT	1.98	0.96
2:B:97(A):GLU:HB2	4:B:513:HOH:O	1.67	0.94
3:C:309:ASP:HB3	3:C:312:ALA:HB3	1.49	0.94
1:A:14(D):ARG:HD2	4:A:475:HOH:O	1.68	0.93
2:B:118:ILE:HD12	4:B:437:HOH:O	1.69	0.93
2:B:87:LYS:HD2	2:B:89:TYR:CD2	2.04	0.93
2:B:41:LEU:CD1	4:B:436:HOH:O	2.17	0.91
2:B:40:LEU:CD2	4:B:637:HOH:O	2.17	0.91
1:A:1(F):GLY:CA	2:B:235:LYS:NZ	2.33	0.90
1:A:1(F):GLY:HA2	2:B:235:LYS:HE2	1.53	0.90
2:B:46:LEU:HD22	2:B:48:SER:O	1.72	0.89
2:B:201:MET:HE2	2:B:210:MET:HG3	1.51	0.89
2:B:204(B):ASN:HD22	2:B:205:ASN:N	1.68	0.89
1:A:14(J):TYR:O	1:A:14(K):ILE:HD12	1.72	0.89
2:B:41:LEU:HD12	4:B:436:HOH:O	1.71	0.89
4:B:628:HOH:O	3:C:311:LEU:HD11	1.74	0.88
1:A:1(E):SER:HA	2:B:123:LEU:O	1.74	0.88
1:A:1(G):PHE:CD1	1:A:1(F):GLY:CA	2.55	0.87
2:B:40:LEU:HD23	4:B:637:HOH:O	1.72	0.87
2:B:139:THR:HG22	2:B:157:VAL:HG22	1.55	0.87
2:B:246:GLY:O	2:B:247:GLU:HB3	1.75	0.86
1:A:1(G):PHE:HA	2:B:123:LEU:HD12	1.58	0.86
2:B:60(B):PRO:HG2	2:B:96:TRP:CE2	2.11	0.86
4:B:628:HOH:O	3:C:311:LEU:CD1	2.23	0.86
1:A:1(H):THR:CG2	1:A:1(G):PHE:N	2.38	0.85
1:A:14(D):ARG:CD	4:A:475:HOH:O	2.27	0.83
1:A:1(G):PHE:HD1	1:A:1(F):GLY:HA3	1.44	0.83
2:B:130:LEU:HD23	2:B:162:ILE:CD1	2.09	0.82
2:B:97(A):GLU:OE2	2:B:175:ARG:NH1	2.12	0.82
2:B:195:ALA:HA	2:B:213:VAL:HG12	1.60	0.82
1:A:1(C):GLU:HG3	2:B:120:PRO:HG2	1.62	0.81
2:B:204(B):ASN:HD22	2:B:204(B):ASN:C	1.78	0.81
2:B:85:LEU:CD1	2:B:106:MET:HE3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HD2	4:A:515:HOH:O	1.81	0.80
2:B:78:ASN:O	4:B:603:HOH:O	2.00	0.80
2:B:138:VAL:HG23	2:B:199:PHE:HD1	1.47	0.80
2:B:187:ARG:NH1	2:B:221:ASP:OD2	2.15	0.80
2:B:60(I):THR:HG22	2:B:62:ASN:HB2	1.63	0.80
1:A:1(F):GLY:CA	2:B:235:LYS:HE2	2.08	0.79
2:B:176:ILE:HG13	4:B:478:HOH:O	1.81	0.79
1:A:1(C):GLU:CB	1:A:1:CYS:HB3	2.12	0.79
2:B:127:GLU:CD	2:B:127:GLU:H	1.88	0.79
2:B:17:VAL:O	2:B:188:GLY:HA2	1.83	0.79
2:B:50:ARG:CD	4:B:607:HOH:O	2.28	0.78
1:A:1(H):THR:HG22	1:A:1(G):PHE:H	1.46	0.78
1:A:10:LYS:O	1:A:12:LEU:HG	1.83	0.78
2:B:31:VAL:HG22	2:B:68:ILE:HG23	1.66	0.78
1:A:1(H):THR:HB	1:A:1(G):PHE:CD2	2.19	0.78
2:B:208:TYR:HB2	2:B:210:MET:HE2	1.64	0.77
2:B:86:GLU:HB3	2:B:107:LYS:HG2	1.67	0.77
2:B:138:VAL:HG23	2:B:199:PHE:CD1	2.20	0.77
2:B:208:TYR:CB	2:B:210:MET:HE2	2.15	0.77
2:B:65:LEU:HD11	2:B:84:MET:HE1	1.65	0.76
1:A:1(H):THR:CG2	1:A:1(G):PHE:HD2	1.98	0.76
2:B:129(B):SER:O	2:B:131:GLN:NE2	2.16	0.76
2:B:78:ASN:C	4:B:603:HOH:O	2.28	0.76
1:A:1(F):GLY:HA3	4:B:421:HOH:O	1.85	0.76
2:B:60(A):TYR:CZ	2:B:60(C):PRO:HG2	2.20	0.76
1:A:10:LYS:CG	1:A:12:LEU:HD12	2.16	0.75
1:A:14(I):SER:CB	2:B:135:LYS:HG3	2.15	0.75
2:B:46:LEU:CD2	2:B:48:SER:O	2.33	0.75
3:C:310:PHE:CD1	3:C:315:GLY:HA3	2.21	0.75
2:B:105:LEU:HD11	2:B:238:ILE:HG23	1.69	0.75
1:A:1(F):GLY:HA2	2:B:235:LYS:HZ1	1.50	0.75
1:A:10:LYS:CG	1:A:12:LEU:CD1	2.64	0.74
4:B:628:HOH:O	3:C:311:LEU:CD2	2.35	0.74
1:A:1(H):THR:HG23	2:B:242:ILE:CD1	2.18	0.74
2:B:164:GLU:HB2	2:B:167:VAL:HG23	1.70	0.74
2:B:35:ARG:O	2:B:38:GLN:HA	1.87	0.73
2:B:60(I):THR:C	2:B:62:ASN:H	1.96	0.73
2:B:95:ASN:HD21	2:B:97(A):GLU:HB3	1.53	0.73
1:A:1(E):SER:CA	2:B:123:LEU:O	2.37	0.73
4:B:628:HOH:O	3:C:311:LEU:HD21	1.87	0.73
2:B:107:LYS:NZ	2:B:246:GLY:HA3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:HD3	2:B:88:ILE:O	1.88	0.73
2:B:169:LYS:NZ	2:B:176:ILE:HG22	2.05	0.72
2:B:110:LYS:O	4:B:440:HOH:O	2.06	0.72
1:A:1(F):GLY:HA2	2:B:235:LYS:HZ3	1.49	0.72
2:B:110:LYS:HB2	4:B:440:HOH:O	1.89	0.72
2:B:147:THR:HB	4:B:454:HOH:O	1.89	0.72
2:B:33:LEU:HD21	2:B:64:LEU:HD23	1.72	0.71
2:B:178:ASP:HB3	2:B:233:ARG:NH1	2.05	0.71
2:B:195:ALA:HA	2:B:213:VAL:O	1.90	0.71
1:A:1(G):PHE:O	1:A:1(D):GLY:N	2.23	0.71
2:B:125:ASP:HB2	2:B:127:GLU:OE2	1.90	0.71
2:B:185:LYS:HB3	2:B:186:PRO:HD2	1.72	0.71
1:A:14(I):SER:HB2	2:B:135:LYS:HG3	1.71	0.71
1:A:14(K):ILE:HG23	4:A:470:HOH:O	1.91	0.71
1:A:14(A):LYS:HG2	2:B:23:GLU:OE2	1.91	0.70
1:A:14(J):TYR:C	1:A:14(K):ILE:HG13	2.15	0.70
2:B:117:TYR:OH	4:B:620:HOH:O	2.07	0.70
1:A:10:LYS:HG3	1:A:12:LEU:HD12	1.72	0.70
2:B:139:THR:CG2	2:B:157:VAL:HG22	2.20	0.70
2:B:87:LYS:CD	2:B:89:TYR:CE2	2.75	0.70
2:B:180:MET:HG2	4:B:448:HOH:O	1.91	0.70
2:B:125:ASP:CG	2:B:127:GLU:OE2	2.36	0.69
2:B:69:GLY:O	2:B:79:ILE:HD11	1.92	0.69
2:B:227:PHE:HE2	4:B:478:HOH:O	1.75	0.69
1:A:1(C):GLU:O	1:A:1(B):ALA:HB2	1.92	0.69
2:B:201:MET:HE3	2:B:210:MET:HG3	1.72	0.69
2:B:35:ARG:NH1	2:B:39:GLU:OE1	2.26	0.69
2:B:187:ARG:NH1	2:B:221:ASP:CG	2.51	0.68
1:A:6:LEU:HA	1:A:10:LYS:HD2	1.74	0.68
2:B:115:SER:O	4:B:409:HOH:O	2.09	0.68
2:B:197:GLY:HA3	4:B:427:HOH:O	1.94	0.68
1:A:1(H):THR:CG2	2:B:242:ILE:HG21	2.23	0.68
1:A:1(H):THR:HG21	2:B:242:ILE:HG21	1.77	0.66
1:A:1(G):PHE:CA	2:B:123:LEU:HD12	2.25	0.66
2:B:204(B):ASN:O	2:B:205:ASN:CB	2.41	0.66
2:B:17:VAL:O	2:B:18:GLU:HB2	1.95	0.66
2:B:201:MET:HE2	2:B:210:MET:CG	2.25	0.66
1:A:1(F):GLY:HA2	2:B:235:LYS:HE3	1.73	0.65
2:B:16:ILE:HD12	2:B:158:VAL:HG12	1.77	0.65
2:B:35:ARG:CB	2:B:39:GLU:HG3	2.26	0.65
2:B:37:PRO:O	2:B:39:GLU:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ASP:O	2:B:112:VAL:HG12	1.95	0.65
2:B:138:VAL:CG2	2:B:199:PHE:HD1	2.09	0.65
2:B:79:ILE:HD12	2:B:79:ILE:O	1.97	0.65
2:B:107:LYS:HZ2	2:B:246:GLY:HA3	1.60	0.65
1:A:1(B):ALA:O	2:B:206:ARG:NH2	2.29	0.65
2:B:65:LEU:HD11	2:B:84:MET:CE	2.26	0.65
3:C:309:ASP:HB3	3:C:312:ALA:CB	2.26	0.65
2:B:204(B):ASN:C	2:B:204(B):ASN:ND2	2.53	0.64
1:A:13:GLU:HB3	1:A:14(C):GLU:CD	2.22	0.64
1:A:13:GLU:HB3	1:A:14(C):GLU:OE1	1.97	0.64
2:B:230:HIS:HB3	2:B:233:ARG:HB2	1.79	0.64
2:B:235:LYS:HE2	2:B:239:GLN:OE1	1.97	0.64
1:A:1(H):THR:HG23	2:B:242:ILE:HD13	1.80	0.64
2:B:63:ASP:HB2	2:B:64:LEU:HD12	1.78	0.63
2:B:81:LYS:HD2	2:B:118:ILE:CD1	2.28	0.63
2:B:137:ARG:HB3	2:B:200:VAL:CG2	2.28	0.63
1:A:1(G):PHE:CD1	4:B:421:HOH:O	2.50	0.63
2:B:79:ILE:HD13	2:B:117:TYR:CG	2.33	0.63
1:A:1(H):THR:HG22	1:A:1(G):PHE:CB	2.29	0.63
2:B:169:LYS:CE	2:B:176:ILE:HG22	2.28	0.63
2:B:201:MET:CG	2:B:210:MET:HG3	2.29	0.63
2:B:60(B):PRO:O	2:B:60(D):TRP:N	2.31	0.62
1:A:1(F):GLY:CA	2:B:235:LYS:HZ3	2.08	0.62
1:A:1(A):ASP:HA	4:B:412:HOH:O	1.99	0.62
1:A:14(C):GLU:OE2	2:B:202:LYS:HE3	1.99	0.62
1:A:1(G):PHE:O	1:A:1(D):GLY:HA2	1.99	0.62
1:A:14(A):LYS:C	1:A:14(B):THR:CG2	2.73	0.62
2:B:137:ARG:O	2:B:199:PHE:HA	2.00	0.62
2:B:57:HIS:C	2:B:57:HIS:CD2	2.77	0.62
2:B:230:HIS:CE1	4:B:434:HOH:O	2.51	0.62
2:B:60(I):THR:O	2:B:62:ASN:N	2.33	0.62
2:B:125:ASP:CB	2:B:127:GLU:OE2	2.47	0.62
2:B:164:GLU:OE2	2:B:167:VAL:HG21	1.99	0.62
2:B:169:LYS:HE3	2:B:176:ILE:CG2	2.30	0.62
2:B:169:LYS:HE3	2:B:176:ILE:HG22	1.80	0.62
2:B:130:LEU:HD23	2:B:162:ILE:HD11	1.80	0.62
1:A:1(H):THR:HG23	2:B:242:ILE:HD12	1.81	0.61
2:B:145:LYS:HE2	4:B:429:HOH:O	1.99	0.61
2:B:146:GLU:HB2	2:B:220:CYS:HB2	1.82	0.61
2:B:35:ARG:HB3	2:B:39:GLU:HG3	1.82	0.61
3:C:310:PHE:CE1	3:C:315:GLY:C	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1(G):PHE:C	2:B:123:LEU:HD12	2.25	0.61
2:B:60(B):PRO:C	2:B:60(D):TRP:H	2.08	0.61
1:A:1(C):GLU:O	4:A:477:HOH:O	2.16	0.61
1:A:1(H):THR:CG2	1:A:1(G):PHE:CD2	2.82	0.61
2:B:18:GLU:HB2	2:B:188:GLY:CA	2.25	0.61
2:B:60(H):PHE:HB3	2:B:63:ASP:OD1	2.00	0.60
2:B:168:CYS:HB3	4:B:478:HOH:O	2.00	0.60
2:B:156:GLN:HG3	4:B:403:HOH:O	2.01	0.60
2:B:35:ARG:HB3	2:B:39:GLU:H	1.66	0.60
2:B:164:GLU:OE2	2:B:185:LYS:NZ	2.33	0.60
1:A:10:LYS:HG2	1:A:12:LEU:HD12	1.82	0.60
1:A:14(J):TYR:C	1:A:14(K):ILE:CG1	2.74	0.60
1:A:14(D):ARG:O	1:A:14(D):ARG:HG3	2.01	0.60
2:B:57:HIS:CE1	3:C:318:ARG:OXT	2.54	0.60
2:B:86:GLU:CB	2:B:107:LYS:HG2	2.32	0.60
2:B:137:ARG:HB3	2:B:200:VAL:HG22	1.84	0.59
2:B:134:TYR:HD1	2:B:134:TYR:N	2.00	0.59
2:B:211:GLY:HA2	2:B:229:THR:O	2.02	0.59
2:B:174:ILE:CD1	3:C:310:PHE:HA	2.32	0.59
1:A:1(G):PHE:HA	2:B:123:LEU:CD1	2.30	0.59
1:A:1(G):PHE:CD1	1:A:1(F):GLY:HA3	2.33	0.59
2:B:131:GLN:O	2:B:132:ALA:C	2.44	0.59
1:A:1(G):PHE:CG	1:A:1(F):GLY:N	2.52	0.58
1:A:9:LYS:HE3	4:A:515:HOH:O	2.02	0.58
3:C:310:PHE:CE1	3:C:315:GLY:HA3	2.38	0.58
2:B:35:ARG:HD3	2:B:39:GLU:CG	2.32	0.58
2:B:60(I):THR:C	2:B:62:ASN:N	2.61	0.58
2:B:195:ALA:CA	2:B:213:VAL:HG12	2.32	0.58
1:A:14(J):TYR:O	1:A:14(K):ILE:CD1	2.48	0.58
2:B:169:LYS:HG2	2:B:176:ILE:HG21	1.84	0.58
2:B:26:MET:SD	2:B:157:VAL:HG21	2.44	0.58
2:B:208:TYR:HB2	2:B:210:MET:CE	2.31	0.58
2:B:99:LEU:HD13	3:C:310:PHE:CE2	2.39	0.58
2:B:134:TYR:N	2:B:134:TYR:CD1	2.72	0.58
2:B:144:LEU:O	2:B:145:LYS:HG3	2.04	0.58
2:B:126:ARG:HG3	4:B:418:HOH:O	2.05	0.57
2:B:164:GLU:OE1	2:B:185:LYS:NZ	2.37	0.57
2:B:178:ASP:O	2:B:233:ARG:HD2	2.04	0.57
2:B:85:LEU:HD21	2:B:106:MET:HE2	1.86	0.57
3:C:316:GLY:O	3:C:317:VAL:C	2.48	0.57
2:B:95:ASN:ND2	2:B:97(A):GLU:HB3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HD13	4:B:436:HOH:O	1.91	0.57
1:A:1(G):PHE:O	1:A:1(D):GLY:CA	2.53	0.57
2:B:85:LEU:HD21	2:B:106:MET:CE	2.35	0.57
1:A:14(A):LYS:C	1:A:14(B):THR:HG23	2.30	0.56
2:B:93:ARG:O	2:B:101:ARG:HD2	2.05	0.56
1:A:1(C):GLU:O	1:A:1(B):ALA:CB	2.52	0.56
1:A:1(C):GLU:HB2	1:A:1:CYS:CB	2.20	0.56
2:B:208:TYR:CB	2:B:210:MET:CE	2.82	0.56
2:B:169:LYS:HZ1	2:B:176:ILE:HG22	1.71	0.56
2:B:29:TRP:O	2:B:45:SER:HA	2.05	0.56
2:B:60(G):ASN:C	4:B:419:HOH:O	2.48	0.56
2:B:57:HIS:CD2	2:B:57:HIS:O	2.59	0.56
2:B:60(B):PRO:HG2	2:B:96:TRP:CZ2	2.41	0.56
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.39	0.56
1:A:1(H):THR:HG22	1:A:1(G):PHE:HB3	1.88	0.55
2:B:60(G):ASN:ND2	4:B:471:HOH:O	2.39	0.55
2:B:172:THR:HA	4:B:407:HOH:O	2.06	0.55
2:B:219:GLY:HA3	2:B:221(A):ARG:NE	2.22	0.55
2:B:61:GLU:OE1	2:B:88:ILE:N	2.39	0.55
2:B:85:LEU:HD11	2:B:106:MET:CE	2.28	0.55
2:B:204(B):ASN:O	2:B:205:ASN:HB3	2.07	0.55
2:B:51:TRP:CH2	2:B:89:TYR:CE1	2.94	0.55
2:B:60(F):LYS:O	2:B:60(G):ASN:HB2	2.06	0.55
2:B:95:ASN:OD1	2:B:95:ASN:C	2.49	0.55
2:B:137:ARG:HD2	2:B:157:VAL:CG1	2.36	0.55
1:A:1(H):THR:CG2	1:A:1(G):PHE:H	2.12	0.55
2:B:87:LYS:HE3	4:B:433:HOH:O	2.06	0.55
2:B:136:GLY:O	2:B:159:ASN:HA	2.06	0.55
1:A:1(H):THR:HG22	1:A:1(G):PHE:CD2	2.42	0.55
2:B:16:ILE:HD11	2:B:138:VAL:HG12	1.89	0.54
2:B:47:ILE:HG21	2:B:123:LEU:HD21	1.89	0.54
2:B:132:ALA:N	4:B:468:HOH:O	2.36	0.54
2:B:204(B):ASN:ND2	2:B:204(B):ASN:N	2.56	0.54
2:B:146:GLU:OE2	2:B:219:GLY:CA	2.56	0.54
2:B:172:THR:HG21	2:B:176:ILE:HD11	1.88	0.54
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HG2	2.42	0.54
2:B:97(A):GLU:HG3	4:B:633:HOH:O	2.07	0.54
2:B:96:TRP:CH2	2:B:97:ARG:HG3	2.43	0.54
2:B:138:VAL:HG21	2:B:228:TYR:CE2	2.42	0.54
2:B:230:HIS:CG	2:B:233:ARG:HG3	2.43	0.54
2:B:165:ARG:CB	2:B:166:PRO:CD	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1(H):THR:CB	1:A:1(G):PHE:CD2	2.90	0.53
2:B:43:GLY:O	2:B:196:GLY:HA3	2.08	0.53
2:B:44:ALA:HB1	2:B:53:LEU:O	2.07	0.53
2:B:98:ASN:N	2:B:98:ASN:OD1	2.41	0.53
2:B:237:TRP:O	2:B:238:ILE:C	2.51	0.53
2:B:63:ASP:C	2:B:64:LEU:HD12	2.34	0.53
2:B:165:ARG:CB	2:B:166:PRO:HD3	2.38	0.53
2:B:174:ILE:HD12	3:C:310:PHE:HA	1.91	0.53
2:B:204(B):ASN:ND2	2:B:204(B):ASN:H	2.07	0.53
1:A:1(H):THR:CB	1:A:1(G):PHE:HD2	2.21	0.53
2:B:74:THR:HG22	2:B:75:ARG:N	2.24	0.53
2:B:29:TRP:CG	2:B:121:VAL:HB	2.44	0.52
2:B:208:TYR:HB3	2:B:210:MET:HE2	1.90	0.52
2:B:164:GLU:CD	2:B:185:LYS:NZ	2.68	0.52
2:B:67:ARG:NE	2:B:80:GLU:OE2	2.32	0.52
3:C:310:PHE:CE1	3:C:315:GLY:CA	2.92	0.52
2:B:235:LYS:HG2	2:B:239:GLN:OE1	2.10	0.52
2:B:87:LYS:CD	2:B:88:ILE:O	2.58	0.52
2:B:60(B):PRO:C	2:B:60(D):TRP:N	2.67	0.52
2:B:132:ALA:CB	2:B:164:GLU:HG3	2.40	0.52
2:B:147:THR:CB	4:B:454:HOH:O	2.51	0.52
2:B:195:ALA:HA	2:B:213:VAL:CG1	2.35	0.52
2:B:85:LEU:CD1	2:B:88:ILE:HD11	2.39	0.51
2:B:187:ARG:NH2	2:B:222:ASP:OD2	2.43	0.51
2:B:203:SER:HB3	2:B:204(B):ASN:HD21	1.75	0.51
2:B:49:ASP:O	2:B:111:PRO:HA	2.10	0.51
2:B:185:LYS:N	2:B:186(B):GLU:OE2	2.39	0.51
2:B:126:ARG:HA	2:B:232:PHE:CZ	2.45	0.51
1:A:14(C):GLU:HB2	4:A:458:HOH:O	2.10	0.51
2:B:235:LYS:O	2:B:239:GLN:HG3	2.11	0.51
2:B:32:MET:HB2	2:B:141:TRP:CZ3	2.46	0.51
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.09	0.51
1:A:1(H):THR:HG22	1:A:1(G):PHE:CA	2.36	0.51
1:A:1(E):SER:N	2:B:123:LEU:O	2.44	0.51
2:B:201:MET:HG2	2:B:210:MET:CG	2.41	0.51
1:A:1(H):THR:HB	1:A:1(G):PHE:HD2	1.67	0.50
1:A:1:CYS:O	2:B:122:CYS:SG	2.69	0.50
1:A:14(A):LYS:O	1:A:14(B):THR:HG22	2.12	0.50
1:A:14(I):SER:OG	2:B:135:LYS:N	2.43	0.50
2:B:18:GLU:HG3	2:B:187:ARG:HG3	1.93	0.50
2:B:185:LYS:HB3	2:B:186:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:CD1	2:B:138:VAL:HG12	2.42	0.50
2:B:107:LYS:HZ2	2:B:246:GLY:CA	2.25	0.50
2:B:93:ARG:HH22	2:B:101:ARG:NH2	2.10	0.50
2:B:152:PRO:HG3	4:B:403:HOH:O	2.11	0.50
2:B:18:GLU:CB	2:B:188:GLY:HA2	2.29	0.49
2:B:46:LEU:HD11	2:B:112:VAL:HG11	1.94	0.49
2:B:185:LYS:HG3	2:B:186(B):GLU:OE2	2.13	0.49
2:B:60(B):PRO:O	2:B:60(E):ASP:N	2.26	0.49
2:B:225:TYR:O	2:B:227:PHE:CD1	2.66	0.49
2:B:59:LEU:HD13	2:B:88:ILE:HG23	1.94	0.49
2:B:85:LEU:HD12	2:B:88:ILE:HD11	1.94	0.49
2:B:166:PRO:HA	4:B:614:HOH:O	2.11	0.49
2:B:201:MET:CG	2:B:210:MET:CG	2.90	0.49
2:B:51:TRP:HH2	2:B:89:TYR:CE1	2.31	0.49
2:B:144:LEU:HD21	2:B:152:PRO:HG3	1.94	0.49
2:B:232:PHE:HB3	4:B:434:HOH:O	2.13	0.49
2:B:195:ALA:CA	2:B:213:VAL:O	2.58	0.49
2:B:36(A):SER:HA	2:B:37:PRO:C	2.38	0.48
2:B:107:LYS:HZ1	2:B:246:GLY:HA3	1.77	0.48
2:B:60(I):THR:HG22	2:B:62:ASN:H	1.78	0.48
2:B:137:ARG:HD3	2:B:159:ASN:OD1	2.14	0.48
2:B:152:PRO:HG3	2:B:156:GLN:HG3	1.94	0.48
2:B:124:PRO:HG3	2:B:210:MET:SD	2.53	0.48
1:A:1(B):ALA:C	2:B:206:ARG:HH22	2.20	0.48
2:B:107:LYS:NZ	2:B:246:GLY:CA	2.77	0.48
2:B:26:MET:O	2:B:26:MET:HG2	2.13	0.48
2:B:51:TRP:CH2	2:B:89:TYR:HE1	2.32	0.48
2:B:125:ASP:OD2	2:B:125:ASP:C	2.56	0.48
2:B:74:THR:CG2	2:B:75:ARG:N	2.76	0.48
2:B:35:ARG:HD3	2:B:39:GLU:HG3	1.96	0.47
2:B:60(I):THR:CG2	2:B:62:ASN:HB2	2.40	0.47
2:B:89:TYR:CE2	4:B:433:HOH:O	2.17	0.47
2:B:206:ARG:NH1	4:B:412:HOH:O	2.29	0.47
1:A:4:ARG:NH2	1:A:8:GLU:OE1	2.41	0.47
2:B:114:PHE:CD1	2:B:114:PHE:N	2.81	0.47
2:B:124:PRO:O	2:B:235:LYS:NZ	2.47	0.47
2:B:137:ARG:O	2:B:200:VAL:N	2.41	0.47
1:A:1(A):ASP:HA	2:B:206:ARG:NH2	2.29	0.47
1:A:14(C):GLU:O	1:A:14(F):LEU:HB2	2.15	0.47
1:A:14(I):SER:OG	2:B:134:TYR:HA	2.15	0.47
1:A:9:LYS:CD	4:A:515:HOH:O	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:HE3	2:B:72:SER:O	2.15	0.47
2:B:169:LYS:CE	2:B:176:ILE:CG2	2.93	0.47
2:B:42:CYS:HB3	2:B:195:ALA:O	2.14	0.47
2:B:101:ARG:HG2	2:B:234:LEU:HD21	1.97	0.47
2:B:129:ALA:O	2:B:130:LEU:HB2	2.15	0.47
1:A:5:PRO:HG2	2:B:116:ASP:HA	1.97	0.46
1:A:1(H):THR:HG23	2:B:242:ILE:HG21	1.95	0.46
1:A:1(E):SER:N	2:B:235:LYS:HZ1	2.13	0.46
2:B:137:ARG:HD2	2:B:157:VAL:HG11	1.97	0.46
2:B:119:HIS:CD2	2:B:120:PRO:HD2	2.51	0.46
2:B:238:ILE:O	2:B:242:ILE:HG13	2.16	0.46
2:B:131:GLN:HB3	4:B:497:HOH:O	2.15	0.46
2:B:208:TYR:HB3	2:B:210:MET:CE	2.45	0.46
2:B:235:LYS:HG2	2:B:239:GLN:CD	2.41	0.46
2:B:100:ASP:O	2:B:101:ARG:HB2	2.16	0.46
2:B:206:ARG:NH1	4:B:498:HOH:O	2.49	0.46
1:A:1(A):ASP:HA	2:B:206:ARG:HH22	1.80	0.45
2:B:36:LYS:HB2	2:B:63:ASP:O	2.16	0.45
2:B:81:LYS:CD	2:B:118:ILE:CD1	2.94	0.45
2:B:32:MET:HE2	2:B:141:TRP:CE3	2.51	0.45
2:B:79:ILE:CD1	2:B:117:TYR:CB	2.95	0.45
2:B:87:LYS:HB3	2:B:89:TYR:CZ	2.51	0.45
2:B:176:ILE:HD13	2:B:176:ILE:H	1.82	0.45
1:A:1(G):PHE:CD1	1:A:1(G):PHE:C	2.87	0.45
1:A:2:GLY:CA	2:B:207:TRP:H	2.30	0.45
2:B:99:LEU:CD1	3:C:310:PHE:CD2	2.99	0.45
2:B:169:LYS:CG	2:B:176:ILE:HG21	2.46	0.45
2:B:140:GLY:HA3	2:B:194:ASP:OD2	2.17	0.44
2:B:201:MET:HE2	2:B:210:MET:CB	2.47	0.44
2:B:169:LYS:HE3	2:B:176:ILE:HB	2.00	0.44
2:B:238:ILE:HD13	2:B:238:ILE:HG21	1.77	0.44
1:A:1(G):PHE:HB2	2:B:239:GLN:HG2	1.99	0.44
2:B:176:ILE:N	2:B:176:ILE:CD1	2.80	0.44
2:B:215:TRP:CD2	3:C:310:PHE:HE2	2.35	0.44
2:B:201:MET:HG2	2:B:210:MET:HG2	1.99	0.44
2:B:244:GLN:NE2	2:B:245:PHE:CE1	2.85	0.44
2:B:87:LYS:HD3	2:B:88:ILE:H	1.83	0.44
2:B:145:LYS:CE	4:B:429:HOH:O	2.61	0.44
2:B:181:PHE:CE2	2:B:210:MET:O	2.71	0.44
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.42	0.43
2:B:232:PHE:CD1	2:B:232:PHE:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:HD13	3:C:310:PHE:CZ	2.53	0.43
1:A:2:GLY:HA2	2:B:207:TRP:H	1.84	0.43
2:B:79:ILE:HD13	2:B:117:TYR:CD1	2.53	0.43
2:B:195:ALA:CB	2:B:213:VAL:O	2.67	0.43
2:B:46:LEU:HD21	2:B:48:SER:O	2.18	0.43
2:B:57:HIS:O	2:B:57:HIS:HD2	2.01	0.43
2:B:16:ILE:HD12	2:B:158:VAL:CG1	2.48	0.43
2:B:236:LYS:HD2	2:B:236:LYS:HA	1.27	0.43
2:B:102:ASP:O	2:B:229:THR:HG21	2.18	0.43
2:B:132:ALA:HB2	2:B:164:GLU:HG3	2.00	0.43
2:B:135:LYS:HA	2:B:161:PRO:HA	2.00	0.43
2:B:137:ARG:HB3	2:B:200:VAL:HG23	2.00	0.42
2:B:60(H):PHE:CG	2:B:64:LEU:HD11	2.54	0.42
2:B:94:TYR:HB2	2:B:101:ARG:O	2.19	0.42
2:B:143:ASN:N	2:B:192:GLU:O	2.43	0.42
1:A:1(H):THR:CG2	2:B:242:ILE:HD12	2.47	0.42
2:B:176:ILE:HD13	2:B:176:ILE:N	2.34	0.42
2:B:36(A):SER:HA	2:B:38:GLN:N	2.34	0.42
2:B:70:LYS:HE3	2:B:70:LYS:HB3	1.51	0.42
2:B:99:LEU:CD1	3:C:310:PHE:CG	3.02	0.42
1:A:1(E):SER:H	2:B:235:LYS:HZ1	1.68	0.42
2:B:151:GLN:HE21	2:B:151:GLN:HB3	1.68	0.42
2:B:89:TYR:OH	2:B:245:PHE:HB3	2.19	0.42
2:B:151:GLN:H	2:B:151:GLN:HG2	0.98	0.42
4:B:616:HOH:O	3:C:308:ACE:H2	2.20	0.41
2:B:242:ILE:C	2:B:244:GLN:H	2.27	0.41
2:B:164:GLU:CD	2:B:185:LYS:HZ3	2.25	0.41
2:B:119:HIS:CG	2:B:120:PRO:HD2	2.55	0.41
2:B:129(C):LEU:HD21	2:B:204:PRO:HD3	2.02	0.41
2:B:144:LEU:C	2:B:145:LYS:HG3	2.45	0.41
2:B:79:ILE:CD1	2:B:117:TYR:HB2	2.50	0.41
2:B:91:HIS:ND1	2:B:91:HIS:C	2.78	0.41
2:B:96:TRP:CZ3	2:B:97:ARG:HG3	2.56	0.41
2:B:130:LEU:HD11	4:B:434:HOH:O	2.21	0.41
2:B:204(B):ASN:HD22	2:B:204(B):ASN:H	1.68	0.40
1:A:14(D):ARG:O	1:A:14(H):GLU:HG3	2.21	0.40
2:B:215:TRP:CE3	3:C:310:PHE:CE2	3.10	0.40
2:B:219:GLY:O	2:B:220:CYS:SG	2.79	0.40
2:B:241:VAL:HA	2:B:244:GLN:HE21	1.86	0.40
3:C:310:PHE:O	3:C:315:GLY:N	2.34	0.40
1:A:1(A):ASP:O	2:B:119:HIS:NE2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:HG23	2:B:158:VAL:HG11	2.03	0.40
2:B:50:ARG:HE	2:B:50:ARG:HB3	1.76	0.40
2:B:78:ASN:HD22	2:B:78:ASN:HA	1.58	0.40
2:B:197:GLY:HA2	2:B:198:PRO:HD3	1.86	0.40
2:B:99:LEU:HD13	3:C:310:PHE:CD2	2.57	0.40
2:B:203:SER:HA	2:B:204:PRO:HD3	1.98	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	31/35 (89%)	22 (71%)	7 (23%)	2 (6%)	1	1
2	B	248/260 (95%)	215 (87%)	28 (11%)	5 (2%)	6	10
3	C	9/11 (82%)	6 (67%)	2 (22%)	1 (11%)	0	0
All	All	288/306 (94%)	243 (84%)	37 (13%)	8 (3%)	4	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(F)	GLY
3	C	309	ASP
1	A	1(B)	ALA
2	B	61	GLU
2	B	77(A)	ARG
2	B	60(C)	PRO
2	B	60(G)	ASN
2	B	38	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	29/30 (97%)	19 (66%)	10 (34%)	0	0
2	B	219/225 (97%)	163 (74%)	56 (26%)	0	1
3	C	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	254/261 (97%)	186 (73%)	68 (27%)	0	1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(H)	THR
1	A	1(G)	PHE
1	A	1(E)	SER
1	A	1(C)	GLU
1	A	1(A)	ASP
1	A	1	CYS
1	A	6	LEU
1	A	9	LYS
1	A	10	LYS
1	A	12	LEU
2	B	27	SER
2	B	33	LEU
2	B	40	LEU
2	B	41	LEU
2	B	46	LEU
2	B	48	SER
2	B	57	HIS
2	B	59	LEU
2	B	60	LEU
2	B	60(A)	TYR
2	B	60(B)	PRO
2	B	60(C)	PRO
2	B	60(D)	TRP
2	B	60(E)	ASP
2	B	60(F)	LYS
2	B	60(G)	ASN

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Mol	Chain	Res	Type
2	B	60(H)	PHE
2	B	60(I)	THR
2	B	61	GLU
2	B	62	ASN
2	B	63	ASP
2	B	65	LEU
2	B	66	VAL
2	B	74	THR
2	B	75	ARG
2	B	79	ILE
2	B	83	SER
2	B	86	GLU
2	B	88	ILE
2	B	90	ILE
2	B	99	LEU
2	B	100	ASP
2	B	107	LYS
2	B	109	LYS
2	B	127	GLU
2	B	128	THR
2	B	137	ARG
2	B	145	LYS
2	B	147	THR
2	B	151	GLN
2	B	154	VAL
2	B	160	LEU
2	B	162	ILE
2	B	165	ARG
2	B	167	VAL
2	B	175	ARG
2	B	176	ILE
2	B	177	THR
2	B	187	ARG
2	B	201	MET
2	B	224	LYS
2	B	231	VAL
2	B	234	LEU
2	B	236	LYS
2	B	241	VAL
2	B	247	GLU
3	C	309	ASP
3	C	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	GLN
2	B	78	ASN
2	B	151	GLN
2	B	204(B)	ASN
2	B	244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.