



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:35 am GMT

PDB ID : 1NRP
Title : CRYSTALLOGRAPHIC STRUCTURES OF THROMBIN COMPLEXED
WITH THROMBIN RECEPTOR PEPTIDES: EXISTENCE OF EX-
PECTED AND NOVEL BINDING MODES
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-01-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

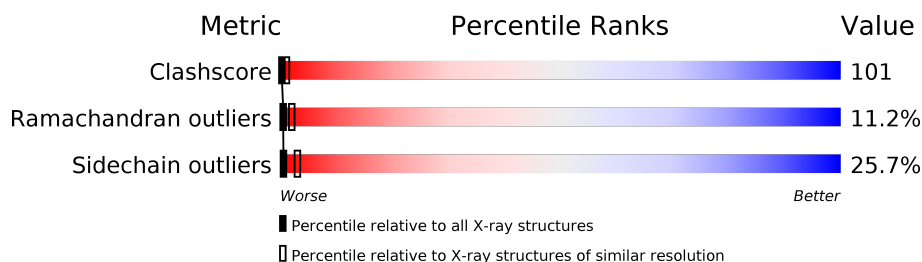
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	R	23	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2445 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			240	149	41	49	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	257	Total	C	N	O	S	0	0	0
			2049	1306	362	367	14			

- Molecule 3 is a protein called RECEPTOR BASED PEPTIDE NR'S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	10	Total	C	N	O	0	0	0
			83	56	11	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	41	HMR	ARG	CONFLICT	UNP P25116

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	61	Total	O	0	0
			61	61		
4	L	11	Total	O	0	0
			11	11		
4	R	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

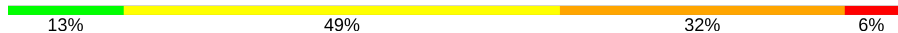
Note EDS was not executed.

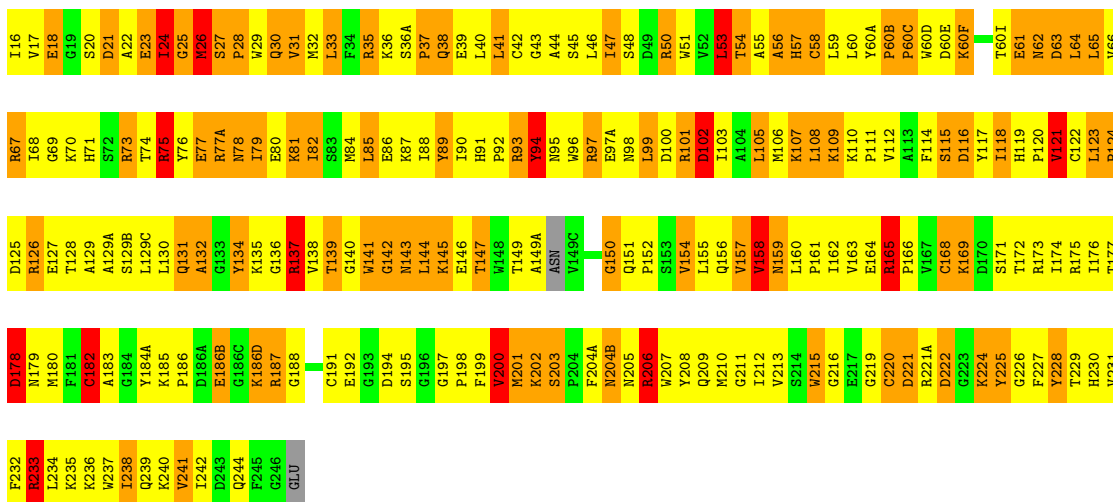
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L:  8% 33% 28% 11% 19%



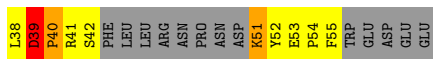
• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H:  13% 49% 32% 6%



• Molecule 3: RECEPTOR BASED PEPTIDE NR'S

Chain R:  30% 9% 57%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.30Å 51.10Å 63.00Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2445	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: HMR

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	L	1.13	0/242	1.78	5/321 (1.6%)
2	H	1.05	2/2101 (0.1%)	2.02	68/2839 (2.4%)
3	R	1.03	0/78	2.40	6/102 (5.9%)
All	All	1.06	2/2421 (0.1%)	2.01	79/3262 (2.4%)

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	L	0	2
2	H	0	4
3	R	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	149(A)	ALA	N-CA	6.46	1.59	1.46
2	H	149	THR	C-N	6.20	1.48	1.34

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	137	ARG	NE-CZ-NH2	-20.60	110.00	120.30
2	H	102	ASP	CB-CG-OD1	10.93	128.14	118.30
2	H	137	ARG	NE-CZ-NH1	10.42	125.51	120.30
3	R	51	LYS	O-C-N	9.54	137.97	122.70
2	H	221	ASP	CB-CG-OD1	9.09	126.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	TYR	CB-CG-CD2	-8.55	115.87	121.00
2	H	102	ASP	CB-CG-OD2	-8.37	110.77	118.30
2	H	184(A)	TYR	CB-CG-CD2	8.27	125.96	121.00
2	H	50	ARG	NE-CZ-NH1	8.17	124.39	120.30
2	H	126	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	H	67	ARG	C-N-CA	7.92	141.50	121.70
2	H	150	GLY	O-C-N	7.87	135.30	122.70
2	H	222	ASP	CB-CG-OD1	-7.44	111.61	118.30
2	H	178	ASP	CA-CB-CG	7.38	129.63	113.40
2	H	187	ARG	NE-CZ-NH2	7.35	123.98	120.30
3	R	51	LYS	CA-C-N	-7.31	101.12	117.20
2	H	97	ARG	NE-CZ-NH2	-7.29	116.66	120.30
3	R	51	LYS	CB-CA-C	-7.24	95.92	110.40
2	H	123	LEU	N-CA-CB	-7.22	95.95	110.40
2	H	93	ARG	NE-CZ-NH2	7.19	123.90	120.30
2	H	221	ASP	CB-CG-OD2	-7.12	111.89	118.30
2	H	233	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	H	97	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	H	60(F)	LYS	O-C-N	6.91	133.75	122.70
3	R	55	PHE	CB-CA-C	6.67	123.75	110.40
2	H	182	CYS	CA-CB-SG	6.63	125.93	114.00
2	H	65	LEU	CB-CA-C	6.56	122.66	110.20
2	H	215	TRP	CA-CB-CG	6.54	126.12	113.70
2	H	101	ARG	NE-CZ-NH2	6.49	123.55	120.30
2	H	222	ASP	CA-C-O	-6.48	106.49	120.10
2	H	30	GLN	N-CA-CB	6.46	122.23	110.60
2	H	105	LEU	CA-CB-CG	6.46	130.15	115.30
2	H	141	TRP	CA-CB-CG	6.43	125.91	113.70
2	H	23	GLU	OE1-CD-OE2	6.42	131.01	123.30
2	H	26	MET	N-CA-CB	-6.36	99.15	110.60
2	H	178	ASP	CB-CG-OD2	6.35	124.02	118.30
2	H	225	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	H	35	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	R	55	PHE	N-CA-C	-6.24	94.14	111.00
2	H	53	LEU	CB-CA-C	6.18	121.95	110.20
2	H	137	ARG	CG-CD-NE	-6.18	98.82	111.80
2	H	126	ARG	CD-NE-CZ	6.16	132.22	123.60
1	L	15	ARG	NE-CZ-NH2	6.15	123.38	120.30
2	H	206	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	H	50	ARG	CD-NE-CZ	6.02	132.03	123.60
2	H	73	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	H	105	LEU	CB-CA-C	5.93	121.47	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	TYR	CB-CG-CD1	5.87	124.52	121.00
2	H	75	ARG	O-C-N	5.87	132.09	122.70
3	R	39	ASP	CA-CB-CG	5.78	126.12	113.40
2	H	75	ARG	NE-CZ-NH2	5.73	123.16	120.30
2	H	124	PRO	C-N-CA	5.60	135.71	121.70
2	H	224	LYS	CA-C-N	-5.58	104.92	117.20
1	L	3	LEU	CB-CA-C	5.51	120.67	110.20
2	H	89	TYR	N-CA-CB	5.51	120.51	110.60
1	L	14(D)	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	H	158	VAL	CA-CB-CG1	5.49	119.13	110.90
2	H	228	TYR	CB-CG-CD1	-5.47	117.72	121.00
2	H	202	LYS	CA-C-O	5.45	131.54	120.10
2	H	121	VAL	CG1-CB-CG2	-5.39	102.27	110.90
2	H	224	LYS	CA-C-O	5.37	131.38	120.10
2	H	56	ALA	CB-CA-C	5.36	118.14	110.10
2	H	168	CYS	CA-CB-SG	5.35	123.63	114.00
2	H	220	CYS	CA-CB-SG	-5.34	104.38	114.00
1	L	1	CYS	CA-CB-SG	-5.29	104.48	114.00
2	H	233	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
2	H	77(A)	ARG	NE-CZ-NH2	5.27	122.94	120.30
2	H	204(A)	PHE	CB-CG-CD1	-5.25	117.12	120.80
2	H	200	VAL	C-N-CA	5.22	134.75	121.70
2	H	132	ALA	N-CA-CB	5.21	117.40	110.10
2	H	35	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
2	H	201	MET	CA-CB-CG	5.20	122.14	113.30
2	H	178	ASP	OD1-CG-OD2	-5.19	113.44	123.30
2	H	203	SER	O-C-N	5.17	130.93	121.10
2	H	175	ARG	O-C-N	5.15	130.94	122.70
2	H	30	GLN	O-C-N	5.14	130.92	122.70
2	H	25	GLY	C-N-CA	5.08	134.41	121.70
2	H	121	VAL	CA-CB-CG1	5.05	118.48	110.90
1	L	15	ARG	NH1-CZ-NH2	-5.04	113.86	119.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	137	ARG	Sidechain
2	H	165	ARG	Sidechain
2	H	75	ARG	Sidechain
2	H	97	ARG	Sidechain
1	L	14(D)	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	15	ARG	Sidechain
3	R	41	HMR	Mainchain,Peptide

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	L	240	0	240	39	0
2	H	2049	0	2000	435	1
3	R	83	0	72	16	1
4	H	61	0	0	0	0
4	L	11	0	0	0	1
4	R	1	0	0	0	0
All	All	2445	0	2312	474	2

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 101.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:TRP:HA	2:H:99:LEU:HD23	1.20	1.17
2:H:36(A):SER:HA	2:H:38:GLN:N	1.60	1.16
1:L:7:PHE:HA	1:L:12:LEU:HB2	1.28	1.15
2:H:86:GLU:CB	2:H:109:LYS:HA	1.81	1.11
2:H:124:PRO:HG3	2:H:210:MET:HE2	1.31	1.11
2:H:59:LEU:HD21	2:H:106:MET:HE2	1.33	1.08
2:H:86:GLU:HB2	2:H:109:LYS:CA	1.84	1.08
2:H:78:ASN:HD22	2:H:78:ASN:N	1.41	1.07
2:H:68:ILE:HB	2:H:81:LYS:HB3	1.37	1.04
2:H:169:LYS:HA	2:H:176:ILE:HD11	1.40	1.03
2:H:224:LYS:HD3	2:H:225:TYR:O	1.59	1.03
2:H:224:LYS:HG2	2:H:225:TYR:H	1.25	1.01
2:H:37:PRO:O	2:H:39:GLU:HG2	1.61	1.01
2:H:77:GLU:HB2	2:H:80:GLU:HB2	1.45	0.98
2:H:47:ILE:HD12	2:H:47:ILE:O	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:39:ASP:OD1	3:R:40:PRO:HD2	1.63	0.96
2:H:24:ILE:HG22	2:H:117:TYR:HE1	1.31	0.96
2:H:68:ILE:O	2:H:81:LYS:N	1.98	0.95
2:H:50:ARG:NH2	2:H:107:LYS:HE3	1.81	0.94
2:H:51:TRP:HE3	2:H:105:LEU:HD11	1.34	0.93
2:H:81:LYS:NZ	2:H:118:ILE:HG21	1.81	0.92
2:H:81:LYS:HZ2	2:H:118:ILE:HG21	1.33	0.92
2:H:197:GLY:O	2:H:213:VAL:HG23	1.69	0.92
2:H:57:HIS:HD2	2:H:58:CYS:N	1.68	0.91
2:H:96:TRP:HA	2:H:99:LEU:CD2	1.99	0.91
2:H:185:LYS:H	2:H:186(B):GLU:HG3	1.34	0.90
2:H:78:ASN:N	2:H:78:ASN:ND2	2.14	0.90
2:H:99:LEU:HD12	3:R:38:LEU:N	1.85	0.90
2:H:41:LEU:H	2:H:41:LEU:HD23	1.37	0.89
1:L:14(G):LEU:HD22	1:L:14(K):ILE:HD11	1.55	0.89
2:H:138:VAL:CG1	2:H:158:VAL:HG12	2.03	0.89
2:H:29:TRP:CD2	2:H:121:VAL:HG23	2.07	0.88
2:H:46:LEU:CD2	2:H:118:ILE:HD12	2.04	0.88
1:L:6:LEU:HD22	2:H:24:ILE:O	1.74	0.87
2:H:138:VAL:HG12	2:H:158:VAL:HG12	1.54	0.87
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.56	0.87
2:H:219:GLY:O	2:H:220:CYS:SG	2.31	0.87
2:H:77(A):ARG:C	2:H:78:ASN:HD22	1.78	0.87
2:H:41:LEU:HD23	2:H:41:LEU:N	1.89	0.86
2:H:59:LEU:HD21	2:H:106:MET:CE	2.04	0.86
1:L:3:LEU:HD13	2:H:206:ARG:HD2	1.58	0.85
2:H:87:LYS:HG3	2:H:88:ILE:O	1.77	0.84
2:H:114:PHE:HA	2:H:118:ILE:HG13	1.58	0.84
2:H:204(B):ASN:HD22	2:H:204(B):ASN:H	1.23	0.84
2:H:99:LEU:CD1	3:R:38:LEU:N	2.40	0.84
2:H:24:ILE:HD13	2:H:24:ILE:H	1.40	0.84
2:H:66:VAL:O	2:H:82:ILE:HA	1.78	0.83
2:H:64:LEU:HD11	2:H:88:ILE:HD11	1.61	0.83
2:H:26:MET:O	2:H:26:MET:HG3	1.78	0.83
2:H:62:ASN:HA	2:H:84:MET:HE1	1.61	0.83
2:H:26:MET:CE	2:H:157:VAL:HG21	2.09	0.82
2:H:94:TYR:HE1	2:H:99:LEU:HD22	1.45	0.82
2:H:24:ILE:HD13	2:H:24:ILE:N	1.93	0.82
2:H:31:VAL:HG23	2:H:68:ILE:HG13	1.61	0.82
2:H:150:GLY:O	2:H:151:GLN:HG2	1.80	0.81
2:H:124:PRO:HG3	2:H:210:MET:CE	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60(B):PRO:HB2	2:H:60(C):PRO:HD3	1.62	0.81
2:H:191:CYS:O	2:H:194:ASP:HB2	1.80	0.81
2:H:224:LYS:CG	2:H:225:TYR:H	1.94	0.81
2:H:50:ARG:HH21	2:H:107:LYS:HE3	1.47	0.80
2:H:206:ARG:HH11	2:H:206:ARG:HG2	1.45	0.79
2:H:51:TRP:CE2	2:H:107:LYS:HG2	2.18	0.79
2:H:62:ASN:HA	2:H:84:MET:CE	2.12	0.79
2:H:85:LEU:HD13	2:H:106:MET:SD	2.21	0.79
2:H:26:MET:HE1	2:H:157:VAL:HG21	1.63	0.78
2:H:71:HIS:NE2	2:H:154:VAL:HG21	1.98	0.78
2:H:51:TRP:HE3	2:H:105:LEU:CD1	1.95	0.78
2:H:171:SER:HB3	2:H:225:TYR:CE2	2.18	0.78
2:H:59:LEU:CD2	2:H:106:MET:HE2	2.14	0.78
2:H:164:GLU:C	2:H:166:PRO:HD2	2.03	0.78
2:H:57:HIS:CD2	2:H:58:CYS:N	2.51	0.78
2:H:73:ARG:O	2:H:73:ARG:HG2	1.85	0.77
2:H:182:CYS:HB2	2:H:226:GLY:O	1.85	0.77
2:H:169:LYS:HE2	2:H:176:ILE:HG13	1.66	0.77
2:H:114:PHE:HA	2:H:118:ILE:CG1	2.14	0.77
2:H:137:ARG:HB2	2:H:159:ASN:HD22	1.48	0.76
2:H:21:ASP:OD1	2:H:21:ASP:N	2.17	0.76
2:H:169:LYS:CA	2:H:176:ILE:HD11	2.14	0.76
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.21	0.76
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.68	0.76
2:H:61:GLU:OE2	2:H:87:LYS:HA	1.86	0.75
2:H:95:ASN:HD22	2:H:97(A):GLU:HB2	1.52	0.75
1:L:13:GLU:HG3	1:L:14(C):GLU:CD	2.07	0.75
2:H:81:LYS:HG2	2:H:112:VAL:CG1	2.16	0.75
2:H:59:LEU:HD23	2:H:88:ILE:HG23	1.69	0.75
2:H:80:GLU:HG2	2:H:81:LYS:N	2.00	0.75
2:H:32:MET:SD	2:H:40:LEU:HD12	2.27	0.74
2:H:233:ARG:O	2:H:236:LYS:HE3	1.86	0.74
2:H:95:ASN:HB2	2:H:100:ASP:OD2	1.87	0.74
2:H:24:ILE:HG22	2:H:117:TYR:CE1	2.20	0.74
2:H:62:ASN:ND2	2:H:62:ASN:H	1.86	0.74
2:H:60:LEU:HD13	2:H:90:ILE:HD12	1.68	0.74
2:H:27:SER:N	2:H:28:PRO:HD3	2.02	0.73
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.69	0.73
2:H:62:ASN:H	2:H:62:ASN:HD22	1.35	0.73
2:H:185:LYS:N	2:H:186(B):GLU:HG3	2.02	0.73
2:H:138:VAL:HG12	2:H:158:VAL:CG1	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ILE:HG21	2:H:53:LEU:HD23	1.70	0.73
2:H:185:LYS:HB3	2:H:186:PRO:HD2	1.71	0.72
3:R:53:GLU:HG2	3:R:54:PRO:CD	2.19	0.72
2:H:36(A):SER:HA	2:H:38:GLN:H	1.53	0.71
1:L:4:ARG:HH22	1:L:14:ASP:HB3	1.54	0.71
2:H:51:TRP:CZ2	2:H:107:LYS:HG2	2.25	0.71
2:H:95:ASN:ND2	2:H:97(A):GLU:HB2	2.05	0.71
2:H:88:ILE:HG12	2:H:106:MET:HG2	1.70	0.71
2:H:89:TYR:HE2	2:H:107:LYS:HB2	1.56	0.71
2:H:103:ILE:HG21	2:H:234:LEU:HD13	1.73	0.71
2:H:60(C):PRO:O	2:H:60(D):TRP:HD1	1.71	0.71
2:H:164:GLU:H	2:H:164:GLU:CD	1.93	0.70
2:H:73:ARG:HD3	2:H:152:PRO:O	1.91	0.70
2:H:169:LYS:HA	2:H:176:ILE:CD1	2.19	0.70
2:H:56:ALA:N	2:H:102:ASP:OD1	2.24	0.70
2:H:185:LYS:HB2	2:H:186(B):GLU:CG	2.22	0.70
1:L:3:LEU:HD11	2:H:205:ASN:OD1	1.91	0.70
2:H:199:PHE:HB3	2:H:211:GLY:HA3	1.74	0.69
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.22	0.69
2:H:86:GLU:HB2	2:H:109:LYS:HA	0.88	0.69
2:H:169:LYS:HG2	2:H:176:ILE:HD11	1.74	0.69
2:H:60:LEU:O	2:H:60:LEU:HD23	1.93	0.69
2:H:60(I):THR:HG22	2:H:63:ASP:OD1	1.92	0.69
2:H:64:LEU:HD13	2:H:85:LEU:CD1	2.23	0.69
2:H:36(A):SER:HA	2:H:37:PRO:C	2.13	0.69
2:H:64:LEU:CD1	2:H:88:ILE:HD11	2.24	0.68
2:H:59:LEU:HD23	2:H:88:ILE:CG2	2.23	0.68
2:H:204(B):ASN:N	2:H:204(B):ASN:HD22	1.92	0.68
2:H:176:ILE:HG22	2:H:180:MET:CE	2.23	0.68
2:H:60(B):PRO:CB	2:H:60(C):PRO:HD3	2.23	0.68
2:H:130:LEU:HD21	2:H:210:MET:HB3	1.74	0.67
3:R:53:GLU:HG2	3:R:54:PRO:HD3	1.76	0.67
2:H:199:PHE:HB3	2:H:211:GLY:CA	2.24	0.67
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.30	0.67
2:H:84:MET:O	2:H:109:LYS:HB3	1.94	0.67
2:H:26:MET:O	2:H:26:MET:CG	2.43	0.67
2:H:179:ASN:O	2:H:230:HIS:HB2	1.96	0.66
2:H:77:GLU:O	2:H:80:GLU:HB3	1.96	0.66
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.30	0.66
2:H:46:LEU:HD23	2:H:118:ILE:HD12	1.78	0.65
2:H:59:LEU:CD2	2:H:88:ILE:HD13	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:206:ARG:HG2	2:H:206:ARG:NH1	2.10	0.65
2:H:29:TRP:O	2:H:45:SER:HA	1.96	0.65
2:H:216:GLY:HA2	2:H:224:LYS:NZ	2.11	0.65
2:H:60(B):PRO:CB	2:H:60(C):PRO:CD	2.74	0.65
2:H:115:SER:O	2:H:117:TYR:N	2.30	0.65
2:H:177:THR:C	2:H:179:ASN:H	2.00	0.65
2:H:32:MET:CE	2:H:70:LYS:HG3	2.27	0.64
2:H:60(D):TRP:CZ2	3:R:52:TYR:O	2.50	0.64
2:H:144:LEU:HD12	2:H:144:LEU:H	1.62	0.64
2:H:81:LYS:HG2	2:H:112:VAL:HG11	1.79	0.64
2:H:46:LEU:HD21	2:H:118:ILE:HD12	1.77	0.64
2:H:224:LYS:HG2	2:H:225:TYR:N	2.06	0.64
2:H:71:HIS:CD2	2:H:154:VAL:HG21	2.31	0.64
3:R:53:GLU:CB	3:R:54:PRO:HD2	2.27	0.64
3:R:53:GLU:CG	3:R:54:PRO:HD2	2.28	0.64
2:H:118:ILE:HG13	2:H:118:ILE:O	1.98	0.64
2:H:27:SER:N	2:H:28:PRO:CD	2.61	0.64
2:H:91:HIS:HE1	2:H:101:ARG:HH11	1.43	0.64
2:H:60(A):TYR:CE1	2:H:60(C):PRO:HG2	2.33	0.64
2:H:69:GLY:HA3	2:H:80:GLU:HA	1.79	0.64
2:H:68:ILE:CB	2:H:81:LYS:HB3	2.22	0.63
2:H:56:ALA:HB1	2:H:94:TYR:CE2	2.33	0.63
2:H:53:LEU:CD1	2:H:212:ILE:HD11	2.28	0.63
2:H:60(B):PRO:HB2	2:H:60(C):PRO:CD	2.27	0.63
2:H:67:ARG:HG2	2:H:82:ILE:HD12	1.80	0.63
2:H:150:GLY:C	2:H:151:GLN:HG2	2.15	0.63
2:H:224:LYS:HE2	2:H:227:PHE:CE1	2.34	0.63
2:H:31:VAL:HG12	2:H:44:ALA:H	1.62	0.63
2:H:53:LEU:HD11	2:H:212:ILE:HD11	1.79	0.63
2:H:64:LEU:HD13	2:H:85:LEU:HD11	1.80	0.63
2:H:51:TRP:CE3	2:H:105:LEU:HD11	2.25	0.63
2:H:136:GLY:O	2:H:159:ASN:HA	1.99	0.63
1:L:3:LEU:HD13	2:H:206:ARG:CD	2.29	0.63
2:H:121:VAL:HG11	2:H:209:GLN:HB2	1.79	0.63
2:H:27:SER:H	2:H:28:PRO:HD3	1.60	0.63
2:H:80:GLU:CG	2:H:81:LYS:N	2.62	0.62
2:H:224:LYS:CG	2:H:225:TYR:N	2.60	0.62
2:H:208:TYR:HB3	2:H:210:MET:CE	2.29	0.62
1:L:13:GLU:HA	1:L:14(C):GLU:OE2	2.00	0.62
2:H:60(B):PRO:O	2:H:60(E):ASP:N	2.29	0.62
2:H:157:VAL:O	2:H:157:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:VAL:HB	2:H:182:CYS:SG	2.40	0.61
1:L:13:GLU:HG3	1:L:14(C):GLU:OE2	2.00	0.61
2:H:81:LYS:HG2	2:H:112:VAL:HG13	1.82	0.61
2:H:121:VAL:CG1	2:H:209:GLN:HB2	2.31	0.61
2:H:17:VAL:HG11	2:H:221:ASP:HB2	1.82	0.61
2:H:230:HIS:HB3	2:H:233:ARG:HB2	1.82	0.61
2:H:94:TYR:CE1	2:H:99:LEU:HD22	2.32	0.61
1:L:14:ASP:OD1	1:L:14:ASP:O	2.19	0.61
2:H:172:THR:OG1	2:H:173:ARG:N	2.32	0.61
2:H:186(D):LYS:HD2	2:H:187:ARG:H	1.65	0.61
1:L:14(F):LEU:O	1:L:14(I):SER:OG	2.16	0.61
3:R:53:GLU:CB	3:R:54:PRO:CD	2.79	0.61
2:H:126:ARG:HA	2:H:129:ALA:HB3	1.82	0.61
2:H:183:ALA:O	2:H:225:TYR:HB3	2.01	0.61
2:H:54:THR:OG1	2:H:55:ALA:N	2.34	0.60
3:R:53:GLU:HG2	3:R:54:PRO:HD2	1.83	0.60
3:R:53:GLU:HB3	3:R:54:PRO:HD2	1.83	0.60
2:H:124:PRO:O	2:H:235:LYS:HE2	2.01	0.60
2:H:24:ILE:N	2:H:24:ILE:CD1	2.61	0.60
1:L:14:ASP:O	1:L:14(C):GLU:HG2	2.01	0.60
2:H:115:SER:O	2:H:118:ILE:N	2.34	0.60
2:H:165:ARG:N	2:H:166:PRO:HD2	2.16	0.60
2:H:177:THR:O	2:H:179:ASN:N	2.35	0.60
2:H:76:TYR:CE2	2:H:77(A):ARG:HA	2.37	0.60
2:H:185:LYS:CB	2:H:186(B):GLU:HG3	2.30	0.59
2:H:31:VAL:CG1	2:H:44:ALA:HB3	2.32	0.59
2:H:234:LEU:O	2:H:238:ILE:HG13	2.03	0.59
2:H:200:VAL:HG13	2:H:209:GLN:HG3	1.83	0.59
2:H:51:TRP:CZ3	2:H:105:LEU:HG	2.38	0.59
2:H:59:LEU:HD21	2:H:88:ILE:HD13	1.85	0.59
2:H:101:ARG:O	2:H:103:ILE:N	2.37	0.58
1:L:6:LEU:CD1	2:H:116:ASP:HB3	2.33	0.58
2:H:94:TYR:HE1	2:H:99:LEU:CD2	2.13	0.58
2:H:85:LEU:CD1	2:H:106:MET:SD	2.89	0.58
2:H:95:ASN:HB2	2:H:100:ASP:CG	2.24	0.58
2:H:154:VAL:HG22	2:H:155:LEU:H	1.69	0.58
2:H:56:ALA:CB	2:H:94:TYR:CE2	2.87	0.58
1:L:8:GLU:C	1:L:10:LYS:H	2.06	0.58
2:H:108:LEU:CD1	2:H:112:VAL:HG23	2.33	0.58
2:H:31:VAL:HG12	2:H:44:ALA:N	2.19	0.57
2:H:232:PHE:O	2:H:235:LYS:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:237:TRP:CZ2	2:H:241:VAL:HG11	2.39	0.57
1:L:3:LEU:HD12	1:L:8:GLU:HG2	1.85	0.57
2:H:24:ILE:CD1	2:H:24:ILE:H	1.97	0.57
2:H:84:MET:O	2:H:109:LYS:CB	2.53	0.57
2:H:171:SER:HB3	2:H:225:TYR:HE2	1.64	0.57
2:H:125:ASP:OD1	2:H:128:THR:CB	2.52	0.57
1:L:3:LEU:HD22	2:H:206:ARG:HE	1.69	0.57
2:H:233:ARG:O	2:H:236:LYS:HG3	2.05	0.57
2:H:206:ARG:CG	2:H:206:ARG:NH1	2.68	0.56
2:H:77(A):ARG:HB3	2:H:78:ASN:ND2	2.20	0.56
2:H:98:ASN:O	2:H:99:LEU:HB2	2.05	0.56
2:H:81:LYS:HZ1	2:H:118:ILE:HG21	1.68	0.56
1:L:8:GLU:OE1	1:L:8:GLU:N	2.39	0.56
2:H:108:LEU:HD12	2:H:112:VAL:HG23	1.87	0.56
1:L:7:PHE:HA	1:L:12:LEU:CB	2.18	0.56
2:H:107:LYS:C	2:H:107:LYS:HD2	2.27	0.55
2:H:136:GLY:HA3	2:H:199:PHE:CE1	2.41	0.55
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ3	2.42	0.55
2:H:95:ASN:CB	2:H:100:ASP:OD2	2.54	0.55
2:H:16:ILE:N	2:H:194:ASP:OD2	2.39	0.55
2:H:171:SER:HB2	2:H:224:LYS:CG	2.37	0.55
2:H:89:TYR:O	2:H:105:LEU:N	2.32	0.55
2:H:90:ILE:HG22	2:H:91:HIS:H	1.72	0.55
2:H:108:LEU:HB3	2:H:110:LYS:O	2.07	0.55
2:H:26:MET:HE2	2:H:157:VAL:HG21	1.86	0.55
2:H:17:VAL:CG2	2:H:220:CYS:HB3	2.37	0.55
2:H:238:ILE:O	2:H:242:ILE:HG13	2.07	0.54
2:H:108:LEU:O	2:H:110:LYS:N	2.41	0.54
2:H:125:ASP:O	2:H:129:ALA:N	2.28	0.54
2:H:129(C):LEU:HD11	2:H:203:SER:HA	1.90	0.54
2:H:138:VAL:CG1	2:H:158:VAL:CG1	2.79	0.54
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.43	0.54
3:R:38:LEU:O	3:R:39:ASP:O	2.25	0.54
2:H:17:VAL:HG21	2:H:220:CYS:HB3	1.90	0.54
2:H:59:LEU:CD2	2:H:106:MET:CE	2.80	0.53
2:H:60(I):THR:O	2:H:63:ASP:HB2	2.08	0.53
2:H:81:LYS:NZ	2:H:81:LYS:HB2	2.22	0.53
1:L:14(M):GLY:C	1:L:15:ARG:HG3	2.28	0.53
2:H:208:TYR:HB3	2:H:210:MET:HE1	1.91	0.53
2:H:65:LEU:CD2	2:H:82:ILE:HD11	2.38	0.53
2:H:59:LEU:CD2	2:H:88:ILE:HG23	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:CYS:C	1:L:3:LEU:H	2.11	0.53
2:H:37:PRO:O	2:H:39:GLU:CG	2.48	0.53
2:H:65:LEU:HD21	2:H:82:ILE:HD11	1.89	0.53
2:H:132:ALA:HB1	2:H:164:GLU:OE2	2.09	0.53
2:H:219:GLY:C	2:H:220:CYS:SG	2.87	0.53
2:H:85:LEU:HD13	2:H:106:MET:CG	2.39	0.53
3:R:53:GLU:CG	3:R:54:PRO:CD	2.84	0.52
2:H:60:LEU:CD1	2:H:90:ILE:HD12	2.37	0.52
2:H:64:LEU:HD13	2:H:85:LEU:HD12	1.91	0.52
2:H:87:LYS:CG	2:H:88:ILE:O	2.56	0.52
2:H:29:TRP:CE3	2:H:121:VAL:HG23	2.43	0.52
2:H:60(A):TYR:N	2:H:60(F):LYS:O	2.42	0.52
2:H:143:ASN:HB2	2:H:192:GLU:HB3	1.91	0.52
2:H:187:ARG:HB2	2:H:221:ASP:OD1	2.10	0.52
2:H:212:ILE:HD12	2:H:231:VAL:HG22	1.91	0.52
2:H:91:HIS:HD2	2:H:237:TRP:CG	2.28	0.52
2:H:152:PRO:HB2	2:H:154:VAL:O	2.10	0.52
2:H:191:CYS:O	2:H:194:ASP:CB	2.54	0.52
2:H:138:VAL:HG13	2:H:158:VAL:HG12	1.89	0.51
1:L:14(G):LEU:HD22	1:L:14(K):ILE:CD1	2.34	0.51
2:H:225:TYR:O	2:H:227:PHE:CE1	2.64	0.51
2:H:31:VAL:HG11	2:H:44:ALA:HB3	1.91	0.51
2:H:33:LEU:HD11	2:H:59:LEU:HD11	1.91	0.51
2:H:31:VAL:O	2:H:43:GLY:HA2	2.10	0.51
2:H:164:GLU:N	2:H:164:GLU:CD	2.63	0.51
2:H:57:HIS:CD2	2:H:57:HIS:C	2.84	0.51
2:H:73:ARG:CG	2:H:73:ARG:O	2.57	0.51
2:H:165:ARG:N	2:H:166:PRO:CD	2.74	0.51
2:H:169:LYS:HE2	2:H:176:ILE:CG1	2.38	0.51
2:H:57:HIS:NE2	2:H:195:SER:HB3	2.26	0.51
2:H:142:GLY:HA2	2:H:192:GLU:O	2.10	0.51
2:H:195:SER:C	2:H:197:GLY:H	2.14	0.51
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.46	0.51
2:H:200:VAL:HG12	2:H:209:GLN:HA	1.93	0.51
2:H:60(C):PRO:O	2:H:60(D):TRP:CD1	2.60	0.51
2:H:176:ILE:HG22	2:H:180:MET:HE1	1.91	0.51
2:H:137:ARG:HE	2:H:159:ASN:HD22	1.58	0.51
2:H:29:TRP:CG	2:H:121:VAL:HG23	2.45	0.50
2:H:68:ILE:O	2:H:80:GLU:HA	2.11	0.50
2:H:125:ASP:OD1	2:H:128:THR:HB	2.11	0.50
2:H:200:VAL:HG12	2:H:209:GLN:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:PRO:CG	2:H:210:MET:HE2	2.22	0.50
2:H:35:ARG:HD3	2:H:39:GLU:CG	2.41	0.50
2:H:94:TYR:HD1	2:H:95:ASN:N	2.10	0.50
2:H:89:TYR:CE2	2:H:107:LYS:HB2	2.43	0.50
2:H:185:LYS:CA	2:H:186(B):GLU:HG3	2.41	0.50
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.94	0.50
2:H:244:GLN:O	2:H:244:GLN:HG2	2.12	0.50
2:H:61:GLU:HG2	2:H:62:ASN:ND2	2.26	0.49
2:H:119:HIS:CD2	2:H:120:PRO:HD2	2.47	0.49
2:H:126:ARG:O	2:H:129(A):ALA:CB	2.60	0.49
2:H:139:THR:HA	2:H:156:GLN:O	2.12	0.49
2:H:60(A):TYR:O	2:H:60(F):LYS:N	2.30	0.49
2:H:129(C):LEU:HB3	2:H:201:MET:SD	2.52	0.49
2:H:35:ARG:N	2:H:39:GLU:O	2.45	0.49
2:H:115:SER:C	2:H:117:TYR:N	2.64	0.49
2:H:125:ASP:O	2:H:126:ARG:C	2.51	0.49
2:H:146:GLU:O	2:H:147:THR:C	2.50	0.49
2:H:59:LEU:HD11	2:H:106:MET:HE2	1.95	0.49
2:H:79:ILE:HG13	2:H:80:GLU:N	2.27	0.49
2:H:71:HIS:CE1	2:H:154:VAL:HG21	2.48	0.49
2:H:121:VAL:HG21	2:H:200:VAL:HG11	1.95	0.48
2:H:126:ARG:O	2:H:129(A):ALA:N	2.46	0.48
2:H:200:VAL:HG12	2:H:209:GLN:N	2.28	0.48
1:L:4:ARG:HG2	2:H:29:TRP:CZ3	2.48	0.48
3:R:38:LEU:C	3:R:39:ASP:O	2.52	0.48
2:H:90:ILE:HG22	2:H:91:HIS:N	2.29	0.48
2:H:200:VAL:CG1	2:H:209:GLN:HA	2.42	0.48
2:H:103:ILE:CG2	2:H:234:LEU:HD13	2.41	0.48
2:H:187:ARG:HH22	2:H:222:ASP:CG	2.16	0.48
2:H:91:HIS:HE1	2:H:101:ARG:HD3	1.78	0.48
2:H:224:LYS:HD3	2:H:225:TYR:C	2.32	0.48
1:L:1:CYS:C	1:L:3:LEU:N	2.65	0.48
2:H:107:LYS:O	2:H:108:LEU:C	2.52	0.48
2:H:46:LEU:HD21	2:H:118:ILE:CD1	2.43	0.48
2:H:115:SER:C	2:H:117:TYR:H	2.16	0.47
2:H:186(D):LYS:HD2	2:H:187:ARG:N	2.27	0.47
2:H:30:GLN:NE2	2:H:198:PRO:HD2	2.29	0.47
2:H:57:HIS:HA	2:H:94:TYR:OH	2.14	0.47
2:H:101:ARG:O	2:H:103:ILE:HG22	2.14	0.47
2:H:108:LEU:CD1	2:H:112:VAL:CG2	2.92	0.47
2:H:230:HIS:CG	2:H:233:ARG:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:183:ALA:HB3	2:H:228:TYR:CE1	2.48	0.47
2:H:101:ARG:HG2	2:H:234:LEU:HD21	1.97	0.47
2:H:74:THR:HG22	2:H:75:ARG:N	2.29	0.47
2:H:26:MET:HE2	2:H:157:VAL:CG2	2.45	0.47
2:H:29:TRP:CD2	2:H:121:VAL:CG2	2.90	0.47
2:H:37:PRO:O	2:H:39:GLU:N	2.47	0.47
2:H:60(I):THR:H	2:H:63:ASP:HB2	1.80	0.47
2:H:119:HIS:CG	2:H:120:PRO:HD2	2.50	0.47
2:H:228:TYR:N	2:H:228:TYR:CD1	2.83	0.47
2:H:81:LYS:HZ2	2:H:81:LYS:HB2	1.79	0.47
2:H:81:LYS:O	2:H:82:ILE:HB	2.15	0.47
2:H:137:ARG:HE	2:H:159:ASN:ND2	2.13	0.47
2:H:64:LEU:CD1	2:H:85:LEU:HD12	2.44	0.47
2:H:169:LYS:HG2	2:H:176:ILE:CD1	2.44	0.47
2:H:32:MET:CE	2:H:70:LYS:HE3	2.45	0.47
2:H:36(A):SER:CA	2:H:37:PRO:C	2.83	0.47
2:H:60(B):PRO:CG	2:H:60(C):PRO:HD3	2.44	0.47
2:H:30:GLN:OE1	2:H:155:LEU:HD11	2.14	0.46
2:H:162:ILE:HD13	2:H:162:ILE:N	2.30	0.46
2:H:182:CYS:SG	2:H:225:TYR:HB2	2.55	0.46
2:H:67:ARG:HA	2:H:81:LYS:O	2.15	0.46
2:H:69:GLY:HA3	2:H:79:ILE:O	2.15	0.46
2:H:96:TRP:CA	2:H:99:LEU:HD23	2.15	0.46
1:L:6:LEU:HD12	2:H:116:ASP:HB3	1.96	0.46
2:H:176:ILE:HG21	2:H:227:PHE:CE2	2.50	0.46
2:H:41:LEU:N	2:H:41:LEU:CD2	2.61	0.46
2:H:70:LYS:HB3	2:H:141:TRP:HZ2	1.81	0.46
2:H:185:LYS:HB2	2:H:186(B):GLU:HG2	1.97	0.46
2:H:204(B):ASN:O	2:H:205:ASN:ND2	2.48	0.46
2:H:51:TRP:CE3	2:H:105:LEU:HG	2.50	0.46
2:H:37:PRO:O	2:H:38:GLN:C	2.54	0.46
2:H:144:LEU:HD12	2:H:144:LEU:N	2.30	0.46
2:H:31:VAL:HG12	2:H:44:ALA:CA	2.46	0.46
2:H:91:HIS:O	2:H:93:ARG:N	2.49	0.46
2:H:51:TRP:CE3	2:H:105:LEU:CD1	2.86	0.45
2:H:230:HIS:CB	2:H:233:ARG:HB2	2.45	0.45
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.68	0.45
2:H:135:LYS:HA	2:H:161:PRO:HA	1.97	0.45
2:H:58:CYS:O	2:H:59:LEU:HD12	2.16	0.45
2:H:32:MET:HE3	2:H:70:LYS:HG3	1.94	0.45
2:H:60(D):TRP:HZ2	3:R:51:LYS:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:225:TYR:O	2:H:227:PHE:CD1	2.69	0.45
2:H:179:ASN:HA	2:H:233:ARG:HD3	1.97	0.45
2:H:71:HIS:CD2	2:H:154:VAL:CG2	3.00	0.45
2:H:108:LEU:C	2:H:110:LYS:N	2.70	0.45
2:H:143:ASN:O	2:H:145:LYS:N	2.49	0.45
2:H:60(B):PRO:C	2:H:60(D):TRP:H	2.20	0.45
2:H:185:LYS:CB	2:H:186:PRO:HD2	2.43	0.44
2:H:27:SER:H	2:H:28:PRO:CD	2.28	0.44
1:L:14(M):GLY:O	1:L:15:ARG:HG3	2.17	0.44
2:H:233:ARG:O	2:H:236:LYS:CG	2.65	0.44
2:H:27:SER:C	2:H:29:TRP:H	2.21	0.44
2:H:125:ASP:O	2:H:128:THR:N	2.51	0.44
1:L:14(M):GLY:HA2	1:L:15:ARG:NH1	2.33	0.44
2:H:32:MET:HE1	2:H:70:LYS:HE3	1.99	0.44
2:H:50:ARG:HB3	2:H:111:PRO:HA	1.99	0.44
2:H:51:TRP:HZ3	2:H:105:LEU:HG	1.78	0.44
2:H:60(C):PRO:C	2:H:60(D):TRP:CD1	2.91	0.44
2:H:62:ASN:ND2	2:H:62:ASN:N	2.62	0.44
3:R:42:SER:O	3:R:51:LYS:HD2	2.18	0.44
2:H:109:LYS:HG2	2:H:110:LYS:HG3	1.99	0.44
2:H:47:ILE:CD1	2:H:47:ILE:O	2.50	0.44
2:H:81:LYS:CG	2:H:112:VAL:HG13	2.47	0.44
2:H:244:GLN:HE21	2:H:244:GLN:HB3	1.35	0.44
2:H:25:GLY:O	2:H:28:PRO:HD3	2.18	0.43
2:H:60(B):PRO:O	2:H:60(D):TRP:N	2.51	0.43
2:H:212:ILE:HG22	2:H:212:ILE:O	2.17	0.43
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.41	0.43
2:H:216:GLY:HA2	2:H:224:LYS:HZ2	1.81	0.43
2:H:216:GLY:HA2	2:H:224:LYS:HZ3	1.81	0.43
2:H:233:ARG:O	2:H:236:LYS:CE	2.62	0.43
2:H:36:LYS:CE	2:H:62:ASN:O	2.66	0.43
1:L:8:GLU:OE2	2:H:207:TRP:NE1	2.47	0.43
2:H:185:LYS:HB3	2:H:186:PRO:CD	2.44	0.43
1:L:5:PRO:HA	1:L:9:LYS:CB	2.37	0.43
1:L:8:GLU:C	1:L:10:LYS:N	2.71	0.43
2:H:18:GLU:OE1	2:H:18:GLU:HA	2.18	0.43
2:H:44:ALA:HB1	2:H:53:LEU:O	2.17	0.43
2:H:164:GLU:C	2:H:166:PRO:CD	2.83	0.43
2:H:16:ILE:HG13	2:H:156:GLN:O	2.19	0.43
2:H:60(B):PRO:HG2	2:H:60(C):PRO:HD3	2.00	0.43
2:H:62:ASN:O	2:H:63:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:THR:C	2:H:179:ASN:N	2.69	0.43
2:H:53:LEU:HD12	2:H:212:ILE:HD11	2.00	0.43
1:L:14(C):GLU:OE1	2:H:202:LYS:NZ	2.51	0.43
2:H:140:GLY:O	2:H:156:GLN:N	2.27	0.42
2:H:185:LYS:H	2:H:186(B):GLU:CG	2.19	0.42
1:L:14(C):GLU:HG3	1:L:14(D):ARG:N	2.34	0.42
1:L:14(J):TYR:HD1	2:H:134:TYR:CD2	2.38	0.42
2:H:204(B):ASN:ND2	2:H:204(B):ASN:N	2.65	0.42
2:H:69:GLY:O	2:H:79:ILE:CD1	2.67	0.42
1:L:14(D):ARG:HG2	1:L:14(D):ARG:O	2.18	0.42
2:H:23:GLU:O	2:H:26:MET:HB3	2.19	0.42
2:H:110:LYS:HA	2:H:111:PRO:HD3	1.85	0.42
2:H:144:LEU:CD1	2:H:144:LEU:H	2.28	0.42
2:H:68:ILE:O	2:H:80:GLU:CA	2.68	0.42
1:L:14:ASP:C	1:L:14:ASP:OD1	2.58	0.42
2:H:60(B):PRO:CG	2:H:60(C):PRO:CD	2.97	0.42
2:H:85:LEU:HD12	2:H:88:ILE:HD11	2.02	0.42
2:H:135:LYS:HG2	2:H:160:LEU:C	2.40	0.42
2:H:85:LEU:HD13	2:H:106:MET:HG2	2.01	0.42
2:H:146:GLU:HA	2:H:220:CYS:HB2	2.01	0.42
2:H:215:TRP:HZ3	2:H:224:LYS:HZ1	1.61	0.42
2:H:191:CYS:N	2:H:194:ASP:OD2	2.38	0.41
2:H:87:LYS:HG3	2:H:88:ILE:N	2.35	0.41
1:L:8:GLU:O	1:L:10:LYS:N	2.53	0.41
2:H:68:ILE:CG2	2:H:118:ILE:HB	2.51	0.41
2:H:141:TRP:O	2:H:152:PRO:HD2	2.20	0.41
2:H:40:LEU:HD23	2:H:40:LEU:O	2.20	0.41
2:H:60(A):TYR:H	2:H:60(F):LYS:HB3	1.86	0.41
2:H:74:THR:HG21	2:H:75:ARG:HH11	1.86	0.41
2:H:108:LEU:O	2:H:109:LYS:C	2.59	0.41
2:H:90:ILE:CG2	2:H:91:HIS:H	2.32	0.41
1:L:14(J):TYR:CD1	2:H:134:TYR:HB3	2.55	0.41
2:H:109:LYS:HD3	2:H:110:LYS:HD2	2.02	0.41
2:H:171:SER:HB2	2:H:224:LYS:HG2	2.03	0.41
2:H:121:VAL:CG2	2:H:200:VAL:HG11	2.51	0.41
2:H:18:GLU:HG3	2:H:187:ARG:HG3	2.03	0.41
2:H:222:ASP:N	2:H:222:ASP:OD1	2.54	0.41
2:H:51:TRP:CE3	2:H:105:LEU:CG	3.04	0.41
1:L:1:CYS:SG	1:L:1:CYS:O	2.77	0.41
2:H:202:LYS:HB2	2:H:207:TRP:CE3	2.56	0.41
2:H:232:PHE:O	2:H:233:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:LEU:C	2:H:109:LYS:HB2	2.41	0.40
2:H:47:ILE:HB	2:H:123:LEU:HD11	2.02	0.40
2:H:163:VAL:CG1	2:H:168:CYS:SG	3.10	0.40
2:H:95:ASN:ND2	2:H:97(A):GLU:CG	2.84	0.40
2:H:65:LEU:HG	2:H:82:ILE:HD11	2.04	0.40
2:H:62:ASN:CA	2:H:84:MET:CE	2.94	0.40
2:H:129(B):SER:O	2:H:131:GLN:NE2	2.55	0.40
2:H:65:LEU:CG	2:H:82:ILE:HD11	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:432:HOH:O	4:L:432:HOH:O[2_756]	0.38	1.82
2:H:75:ARG:CG	3:R:53:GLU:OE1[4_645]	2.13	0.07

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	L	27/36 (75%)	13 (48%)	6 (22%)	8 (30%)	0	0
2	H	253/259 (98%)	175 (69%)	55 (22%)	23 (9%)	1	4
3	R	5/23 (22%)	2 (40%)	2 (40%)	1 (20%)	0	0
All	All	285/318 (90%)	190 (67%)	63 (22%)	32 (11%)	0	2

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1	CYS
1	L	10	LYS
1	L	14(A)	LYS

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Mol	Chain	Res	Type
1	L	14(L)	ASP
2	H	22	ALA
2	H	24	ILE
2	H	116	ASP
2	H	178	ASP
1	L	9	LYS
1	L	11	SER
1	L	14(M)	GLY
2	H	37	PRO
2	H	92	PRO
2	H	109	LYS
2	H	142	GLY
2	H	144	LEU
2	H	238	ILE
1	L	2	GLY
2	H	18	GLU
2	H	60(C)	PRO
2	H	75	ARG
2	H	147	THR
2	H	38	GLN
2	H	108	LEU
2	H	28	PRO
2	H	77	GLU
2	H	102	ASP
2	H	186(B)	GLU
2	H	27	SER
2	H	60(B)	PRO
3	R	39	ASP
2	H	82	ILE

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	L	27/31 (87%)	17 (63%)	10 (37%)	0	1
2	H	217/225 (96%)	163 (75%)	54 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	9/22 (41%)	8 (89%)	1 (11%)	7	28
All	All	253/278 (91%)	188 (74%)	65 (26%)	0	3

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	8	GLU
1	L	10	LYS
1	L	14	ASP
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(E)	GLU
1	L	14(G)	LEU
1	L	14(K)	ILE
1	L	14(L)	ASP
2	H	20	SER
2	H	21	ASP
2	H	24	ILE
2	H	26	MET
2	H	31	VAL
2	H	33	LEU
2	H	41	LEU
2	H	42	CYS
2	H	47	ILE
2	H	48	SER
2	H	53	LEU
2	H	54	THR
2	H	57	HIS
2	H	58	CYS
2	H	61	GLU
2	H	62	ASN
2	H	63	ASP
2	H	64	LEU
2	H	78	ASN
2	H	79	ILE
2	H	81	LYS
2	H	85	LEU
2	H	94	TYR
2	H	99	LEU
2	H	107	LYS
2	H	115	SER

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Mol	Chain	Res	Type
2	H	118	ILE
2	H	121	VAL
2	H	122	CYS
2	H	127	GLU
2	H	131	GLN
2	H	134	TYR
2	H	139	THR
2	H	143	ASN
2	H	145	LYS
2	H	154	VAL
2	H	157	VAL
2	H	158	VAL
2	H	159	ASN
2	H	165	ARG
2	H	169	LYS
2	H	174	ILE
2	H	178	ASP
2	H	182	CYS
2	H	186(D)	LYS
2	H	200	VAL
2	H	204(B)	ASN
2	H	206	ARG
2	H	221(A)	ARG
2	H	229	THR
2	H	233	ARG
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL
3	R	40	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	57	HIS
2	H	62	ASN
2	H	78	ASN
2	H	91	HIS
2	H	95	ASN
2	H	159	ASN
2	H	204(B)	ASN
2	H	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HMR	R	41	3	5,5,12	1.43	1 (20%)	4,5,14	2.39	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HMR	R	41	3	-	0/3/3/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	41	HMR	CH2-CA	-2.10	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	41	HMR	O-C-CH2	-3.43	114.39	125.48
3	R	41	HMR	CB-CA-CH2	-2.88	108.68	111.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.