Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:10 PM GMT

PDB ID	:	1NRS
Title	:	CRYSTALLOGRAPHIC STRUCTURES OF THROMBIN COMPLEXED WITH THROMBIN RECEPTOR PEPTIDES: EXISTENCE OF EXPECTED AND NOVEL BINDING MODES
Authors	:	Tulinsky, A.; Mathews, I.I.
Deposited on	:	1994-01-18
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

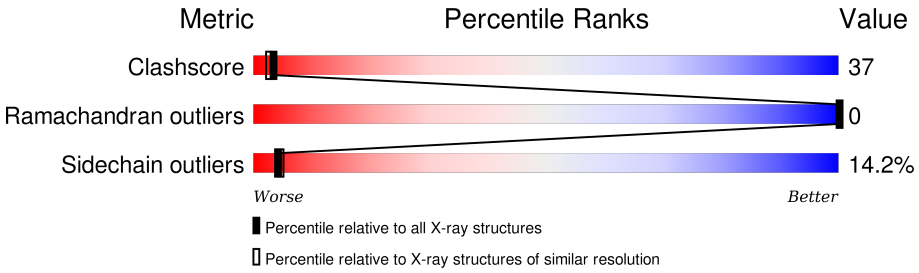
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	L	36	33% 25% 11% 6% 25%
2	H	259	22% 46% 24% 5% •
3	R	4	25% 50% 25%
4	I	12	8% 50% 8% 8% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2573 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	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2029	1293	359	363	14			

- Molecule 3 is a protein called RECEPTOR BASED PEPTIDE NRP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	4	Total	C	N	O	0	0	0
			34	21	7	6			

- Molecule 4 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	9	Total	C	N	O	S	0	0	0
			78	49	9	19	1			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	20	Total	O	0	0
			20	20		
5	H	177	Total	O	0	0
			177	177		
5	R	5	Total	O	0	0
			5	5		
5	I	8	Total	O	0	0
			8	8		

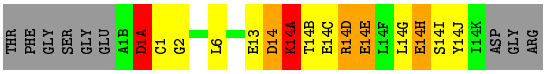
3 Residue-property plots (i)

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.

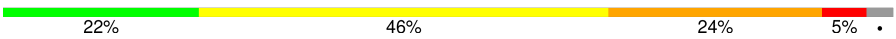
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

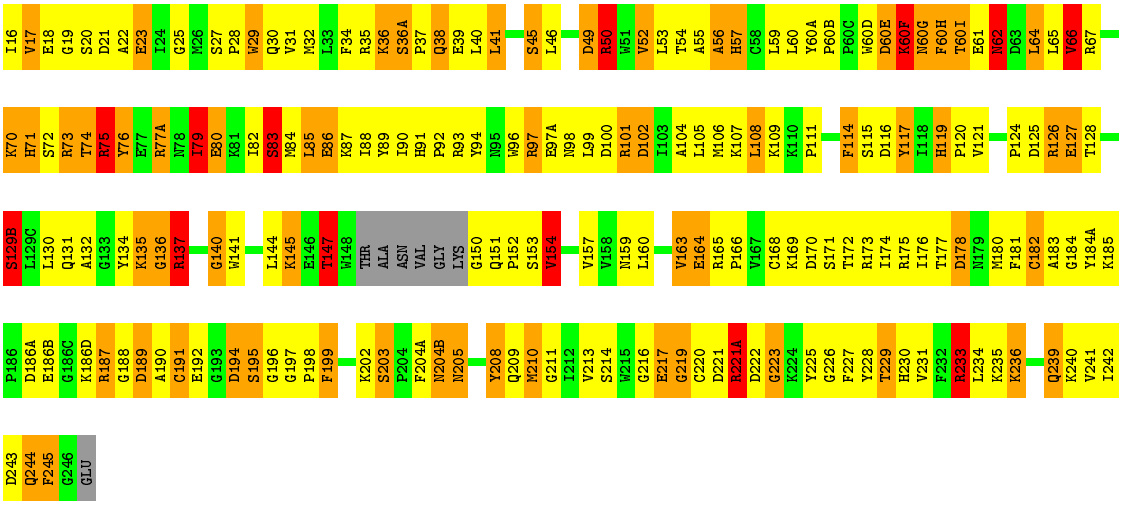
Chain L:



- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

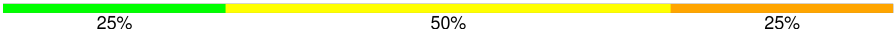
Chain H:





- Molecule 3: RECEPTOR BASED PEPTIDE NRP

Chain R:



- Molecule 4: HIRUGEN

Chain I:


ASN
GLY
D55
F56
E57
E58
I59
P60
E61
E62
Y63
LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.00Å 72.40Å 72.80Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2573	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: TYS

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	1.96	4/224 (1.8%)	2.95	21/298 (7.0%)
2	H	1.93	35/2081 (1.7%)	3.00	194/2812 (6.9%)
3	R	2.19	0/34	3.04	4/45 (8.9%)
4	I	1.10	0/63	2.62	6/85 (7.1%)
All	All	1.92	39/2402 (1.6%)	2.98	225/3240 (6.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	45	SER	CB-OG	9.11	1.54	1.42
2	H	203	SER	CB-OG	7.90	1.52	1.42
1	L	14(I)	SER	CB-OG	7.73	1.52	1.42
2	H	197	GLY	C-O	7.34	1.35	1.23
2	H	208	TYR	CG-CD2	7.17	1.48	1.39
1	L	14(D)	ARG	CZ-NH2	6.67	1.41	1.33
2	H	115	SER	C-O	6.64	1.35	1.23
2	H	54	THR	CB-OG1	6.60	1.56	1.43
2	H	219	GLY	N-CA	6.51	1.55	1.46
2	H	130	LEU	N-CA	6.40	1.59	1.46
2	H	164	GLU	CD-OE2	6.24	1.32	1.25
2	H	36(A)	SER	CB-OG	6.17	1.50	1.42
2	H	94	TYR	CG-CD2	6.13	1.47	1.39
2	H	195	SER	CB-OG	6.03	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	223	GLY	N-CA	-5.99	1.37	1.46
2	H	196	GLY	N-CA	5.95	1.54	1.46
1	L	2	GLY	C-N	5.84	1.47	1.34
2	H	120	PRO	C-O	5.73	1.34	1.23
2	H	28	PRO	C-O	5.68	1.34	1.23
2	H	223	GLY	C-O	5.60	1.32	1.23
2	H	231	VAL	C-O	5.57	1.33	1.23
2	H	209	GLN	C-O	5.57	1.33	1.23
2	H	178	ASP	CB-CG	5.55	1.63	1.51
2	H	168	CYS	C-O	5.54	1.33	1.23
2	H	216	GLY	N-CA	5.51	1.54	1.46
2	H	140	GLY	N-CA	5.44	1.54	1.46
1	L	14(H)	GLU	CD-OE1	5.42	1.31	1.25
2	H	219	GLY	C-O	5.41	1.32	1.23
2	H	169	LYS	C-O	5.38	1.33	1.23
2	H	30	GLN	C-O	5.33	1.33	1.23
2	H	119	HIS	C-O	5.33	1.33	1.23
2	H	46	LEU	C-O	5.29	1.33	1.23
2	H	182	CYS	N-CA	5.28	1.56	1.46
2	H	217	GLU	CB-CG	5.27	1.62	1.52
2	H	89	TYR	C-O	5.21	1.33	1.23
2	H	82	ILE	C-O	5.20	1.33	1.23
2	H	54	THR	N-CA	5.16	1.56	1.46
2	H	229	THR	C-O	5.05	1.32	1.23
2	H	182	CYS	C-O	5.02	1.32	1.23

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	126	ARG	NE-CZ-NH2	28.93	134.76	120.30
2	H	187	ARG	NE-CZ-NH1	27.55	134.07	120.30
1	L	14(D)	ARG	NE-CZ-NH1	23.05	131.82	120.30
2	H	221(A)	ARG	NE-CZ-NH2	-21.52	109.54	120.30
2	H	50	ARG	NE-CZ-NH1	21.26	130.93	120.30
2	H	187	ARG	NE-CZ-NH2	-19.71	110.44	120.30
2	H	97	ARG	NE-CZ-NH2	-17.05	111.78	120.30
2	H	50	ARG	NE-CZ-NH2	-16.92	111.84	120.30
2	H	93	ARG	NE-CZ-NH1	15.48	128.04	120.30
2	H	94	TYR	CB-CG-CD2	-14.46	112.32	121.00
2	H	125	ASP	CB-CG-OD1	-13.80	105.88	118.30
2	H	117	TYR	CB-CG-CD2	-13.62	112.83	121.00
2	H	126	ARG	NE-CZ-NH1	-13.30	113.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	228	TYR	CB-CG-CD2	13.20	128.92	121.00
2	H	94	TYR	CB-CG-CD1	12.80	128.68	121.00
2	H	116	ASP	CB-CG-OD1	12.78	129.80	118.30
2	H	208	TYR	CB-CG-CD2	-12.65	113.41	121.00
2	H	184(A)	TYR	CB-CG-CD2	12.34	128.40	121.00
1	L	14(D)	ARG	NE-CZ-NH2	-12.30	114.15	120.30
2	H	117	TYR	CB-CG-CD1	12.00	128.20	121.00
2	H	175	ARG	NE-CZ-NH1	-11.64	114.48	120.30
2	H	221(A)	ARG	NE-CZ-NH1	11.61	126.11	120.30
2	H	173	ARG	NE-CZ-NH1	11.55	126.07	120.30
2	H	102	ASP	CB-CG-OD1	-11.36	108.08	118.30
2	H	233	ARG	NE-CZ-NH1	11.27	125.94	120.30
2	H	184(A)	TYR	CB-CG-CD1	-10.95	114.43	121.00
2	H	208	TYR	CB-CG-CD1	10.84	127.50	121.00
2	H	67	ARG	NE-CZ-NH1	10.52	125.56	120.30
3	R	39	ASP	CB-CG-OD1	-10.19	109.13	118.30
2	H	66	VAL	CA-CB-CG1	10.17	126.15	110.90
2	H	73	ARG	NE-CZ-NH1	9.96	125.28	120.30
2	H	170	ASP	CB-CG-OD1	9.80	127.12	118.30
2	H	97	ARG	CD-NE-CZ	-9.68	110.05	123.60
1	L	14(A)	LYS	N-CA-CB	9.59	127.85	110.60
2	H	221(A)	ARG	CD-NE-CZ	-9.51	110.29	123.60
2	H	233	ARG	CD-NE-CZ	9.49	136.89	123.60
2	H	97	ARG	NE-CZ-NH1	9.39	124.99	120.30
2	H	221	ASP	CB-CG-OD1	9.37	126.73	118.30
2	H	67	ARG	NH1-CZ-NH2	-9.22	109.25	119.40
2	H	178	ASP	CB-CG-OD2	-9.02	110.18	118.30
2	H	60(H)	PHE	C-N-CA	8.87	143.88	121.70
2	H	130	LEU	CB-CA-C	8.71	126.74	110.20
2	H	101	ARG	NE-CZ-NH1	8.70	124.65	120.30
2	H	154	VAL	N-CA-CB	-8.63	92.50	111.50
3	R	39	ASP	CB-CG-OD2	8.59	126.03	118.30
2	H	225	TYR	CD1-CE1-CZ	-8.38	112.25	119.80
2	H	225	TYR	CB-CG-CD1	-8.36	115.98	121.00
2	H	83	SER	N-CA-CB	8.05	122.57	110.50
1	L	14(H)	GLU	OE1-CD-OE2	7.93	132.82	123.30
2	H	154	VAL	CB-CA-C	7.91	126.43	111.40
2	H	67	ARG	CD-NE-CZ	7.89	134.64	123.60
2	H	194	ASP	CB-CG-OD2	7.87	125.39	118.30
2	H	55	ALA	N-CA-CB	-7.75	99.25	110.10
2	H	75	ARG	NE-CZ-NH2	7.74	124.17	120.30
2	H	225	TYR	CB-CG-CD2	7.74	125.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	57	GLU	OE1-CD-OE2	7.71	132.56	123.30
2	H	163	VAL	CA-CB-CG1	7.71	122.47	110.90
2	H	186(D)	LYS	CA-CB-CG	7.70	130.35	113.40
3	R	41	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	H	114	PHE	CB-CG-CD1	-7.67	115.43	120.80
2	H	147	THR	O-C-N	7.67	134.98	122.70
2	H	60(I)	THR	CA-CB-CG2	7.66	123.13	112.40
2	H	60(I)	THR	CA-CB-OG1	-7.63	92.98	109.00
2	H	127	GLU	OE1-CD-OE2	-7.62	114.15	123.30
2	H	137	ARG	NE-CZ-NH1	7.61	124.10	120.30
2	H	41	LEU	N-CA-CB	-7.60	95.21	110.40
2	H	151	GLN	CB-CA-C	7.46	125.33	110.40
2	H	60(D)	TRP	O-C-N	7.46	134.63	122.70
2	H	67	ARG	NE-CZ-NH2	7.44	124.02	120.30
2	H	60(E)	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	L	1(A)	ASP	CB-CA-C	7.37	125.13	110.40
2	H	129(B)	SER	CA-C-O	-7.31	104.76	120.10
2	H	130	LEU	N-CA-CB	-7.28	95.85	110.40
1	L	1(A)	ASP	CB-CG-OD2	-7.26	111.76	118.30
2	H	173	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	H	187	ARG	CD-NE-CZ	7.20	133.68	123.60
2	H	180	MET	O-C-N	7.19	134.20	122.70
2	H	228	TYR	CB-CG-CD1	-7.17	116.70	121.00
2	H	126	ARG	NH1-CZ-NH2	-7.12	111.57	119.40
2	H	41	LEU	CB-CA-C	7.06	123.61	110.20
2	H	31	VAL	CA-C-N	7.03	132.67	117.20
2	H	178	ASP	O-C-N	7.03	133.94	122.70
2	H	227	PHE	CB-CG-CD2	-6.97	115.92	120.80
4	I	62	GLU	CA-CB-CG	6.97	128.73	113.40
2	H	55	ALA	CB-CA-C	6.93	120.49	110.10
2	H	147	THR	N-CA-CB	6.87	123.34	110.30
2	H	60(H)	PHE	CB-CG-CD1	-6.83	116.02	120.80
2	H	194	ASP	O-C-N	-6.81	111.80	122.70
2	H	101	ARG	NE-CZ-NH2	-6.75	116.92	120.30
2	H	38	GLN	CA-C-O	-6.74	105.94	120.10
2	H	114	PHE	CD1-CE1-CZ	-6.71	112.04	120.10
2	H	38	GLN	CB-CG-CD	6.69	129.00	111.60
2	H	130	LEU	O-C-N	-6.69	111.99	122.70
2	H	176	ILE	CA-CB-CG2	6.66	124.22	110.90
2	H	22	ALA	N-CA-CB	-6.64	100.81	110.10
2	H	80	GLU	CA-CB-CG	6.61	127.93	113.40
2	H	97(A)	GLU	CG-CD-OE2	-6.61	105.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	14(D)	ARG	CD-NE-CZ	6.60	132.84	123.60
2	H	141	TRP	O-C-N	6.49	134.23	123.20
2	H	31	VAL	O-C-N	-6.47	112.36	122.70
2	H	38	GLN	CA-CB-CG	6.44	127.57	113.40
2	H	172	THR	N-CA-CB	-6.43	98.09	110.30
2	H	204(A)	PHE	CA-CB-CG	-6.41	98.51	113.90
1	L	1(A)	ASP	O-C-N	6.37	132.89	122.70
2	H	60	LEU	CB-CG-CD2	-6.34	100.22	111.00
2	H	205	ASN	CB-CA-C	6.33	123.05	110.40
2	H	189	ASP	CB-CG-OD1	6.28	123.95	118.30
2	H	98	ASN	O-C-N	6.26	132.72	122.70
2	H	213	VAL	CA-C-O	6.25	133.24	120.10
2	H	222	ASP	CB-CG-OD2	-6.22	112.70	118.30
2	H	30	GLN	CA-CB-CG	-6.22	99.72	113.40
2	H	79	ILE	CB-CA-C	6.21	124.03	111.60
2	H	60(G)	ASN	O-C-N	6.21	132.64	122.70
2	H	38	GLN	O-C-N	6.20	132.62	122.70
2	H	19	GLY	CA-C-O	6.17	131.72	120.60
2	H	124	PRO	CA-C-O	6.17	135.01	120.20
2	H	93	ARG	NH1-CZ-NH2	-6.17	112.62	119.40
2	H	85	LEU	CA-CB-CG	-6.10	101.26	115.30
2	H	60(A)	TYR	CB-CG-CD1	-6.10	117.34	121.00
2	H	66	VAL	O-C-N	-6.08	112.98	122.70
2	H	84	MET	CG-SD-CE	-6.07	90.48	100.20
2	H	126	ARG	CD-NE-CZ	-6.07	115.10	123.60
2	H	86	GLU	CG-CD-OE1	6.07	130.44	118.30
2	H	153	SER	N-CA-CB	6.02	119.53	110.50
2	H	147	THR	CA-CB-CG2	6.01	120.81	112.40
1	L	14(E)	GLU	CG-CD-OE2	6.00	130.29	118.30
2	H	184(A)	TYR	N-CA-CB	-5.96	99.88	110.60
2	H	181	PHE	CG-CD1-CE1	-5.94	114.27	120.80
1	L	14(I)	SER	N-CA-CB	5.90	119.36	110.50
2	H	125	ASP	OD1-CG-OD2	5.90	134.52	123.30
2	H	56	ALA	N-CA-CB	5.90	118.36	110.10
2	H	97	ARG	N-CA-CB	5.90	121.22	110.60
2	H	70	LYS	CD-CE-NZ	-5.85	98.24	111.70
4	I	57	GLU	CG-CD-OE2	-5.85	106.61	118.30
1	L	14(D)	ARG	C-N-CA	5.84	136.31	121.70
2	H	129(B)	SER	CB-CA-C	-5.84	99.00	110.10
2	H	27	SER	CB-CA-C	-5.84	99.00	110.10
2	H	137	ARG	O-C-N	5.83	132.02	122.70
2	H	181	PHE	CZ-CE2-CD2	-5.82	113.11	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	71	HIS	CA-CB-CG	-5.81	103.72	113.60
2	H	77(A)	ARG	O-C-N	-5.78	113.45	122.70
2	H	30	GLN	N-CA-CB	-5.76	100.23	110.60
2	H	126	ARG	CG-CD-NE	-5.76	99.71	111.80
2	H	177	THR	CA-C-O	5.75	132.17	120.10
2	H	221(A)	ARG	CA-CB-CG	-5.72	100.81	113.40
2	H	31	VAL	CA-CB-CG1	-5.72	102.32	110.90
2	H	171	SER	N-CA-CB	5.71	119.07	110.50
2	H	180	MET	CA-C-O	-5.71	108.10	120.10
1	L	1	CYS	CA-CB-SG	5.71	124.28	114.00
2	H	86	GLU	CG-CD-OE2	-5.69	106.92	118.30
2	H	52	VAL	C-N-CA	5.65	135.81	121.70
2	H	57	HIS	CA-CB-CG	-5.62	104.04	113.60
2	H	60(E)	ASP	CA-CB-CG	-5.60	101.07	113.40
2	H	97	ARG	O-C-N	5.59	131.65	122.70
2	H	83	SER	CA-C-N	-5.59	104.91	117.20
2	H	45	SER	N-CA-CB	5.58	118.87	110.50
2	H	21	ASP	CB-CG-OD2	-5.56	113.29	118.30
2	H	73	ARG	CD-NE-CZ	5.54	131.36	123.60
2	H	199	PHE	CB-CA-C	5.54	121.48	110.40
2	H	101	ARG	CD-NE-CZ	-5.54	115.85	123.60
2	H	67	ARG	CG-CD-NE	5.53	123.42	111.80
2	H	97	ARG	CA-C-O	-5.53	108.49	120.10
2	H	217	GLU	CA-C-N	-5.53	105.15	116.20
2	H	115	SER	N-CA-CB	-5.51	102.23	110.50
4	I	62	GLU	N-CA-CB	5.51	120.52	110.60
2	H	213	VAL	O-C-N	-5.50	113.90	122.70
2	H	97	ARG	CA-CB-CG	-5.49	101.31	113.40
2	H	59	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	L	14(H)	GLU	CA-CB-CG	-5.49	101.33	113.40
2	H	190	ALA	N-CA-CB	5.46	117.75	110.10
2	H	60(F)	LYS	CG-CD-CE	5.46	128.28	111.90
2	H	49	ASP	CB-CG-OD2	-5.44	113.41	118.30
2	H	62	ASN	N-CA-C	5.43	125.67	111.00
2	H	124	PRO	CA-C-N	-5.43	105.26	117.20
2	H	84	MET	CA-CB-CG	-5.41	104.11	113.30
1	L	14(B)	THR	CA-C-O	-5.40	108.77	120.10
2	H	244	GLN	O-C-N	5.40	131.34	122.70
2	H	98	ASN	CA-C-O	-5.37	108.83	120.10
2	H	108	LEU	CB-CA-C	5.37	120.39	110.20
2	H	71	HIS	CA-C-O	5.36	131.36	120.10
4	I	62	GLU	OE1-CD-OE2	-5.36	116.87	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	59	ILE	O-C-N	5.33	131.22	121.10
3	R	41	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	H	29	TRP	CE3-CZ3-CH2	-5.32	115.35	121.20
1	L	13	GLU	CA-CB-CG	5.31	125.08	113.40
2	H	190	ALA	N-CA-C	-5.30	96.68	111.00
2	H	141	TRP	CB-CG-CD2	-5.30	119.72	126.60
2	H	198	PRO	CB-CA-C	-5.30	98.76	112.00
2	H	136	GLY	N-CA-C	-5.29	99.87	113.10
2	H	104	ALA	CA-C-N	-5.28	105.59	117.20
2	H	150	GLY	O-C-N	5.27	131.13	122.70
2	H	25	GLY	CA-C-O	-5.26	111.13	120.60
2	H	225	TYR	CG-CD1-CE1	5.26	125.51	121.30
2	H	23	GLU	CA-CB-CG	5.26	124.97	113.40
2	H	17	VAL	CA-C-O	5.25	131.12	120.10
2	H	205	ASN	CB-CG-OD1	5.24	132.09	121.60
2	H	116	ASP	CB-CG-OD2	-5.24	113.59	118.30
2	H	144	LEU	CB-CG-CD1	-5.23	102.10	111.00
2	H	85	LEU	CB-CG-CD2	-5.22	102.13	111.00
2	H	60(D)	TRP	N-CA-CB	5.21	119.99	110.60
2	H	191	CYS	O-C-N	5.21	131.04	122.70
2	H	77(A)	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	H	59	LEU	CB-CG-CD1	5.18	119.80	111.00
1	L	13	GLU	CA-C-N	5.18	128.59	117.20
1	L	14	ASP	CB-CG-OD2	5.17	122.95	118.30
2	H	126	ARG	CB-CG-CD	-5.17	98.17	111.60
2	H	128	THR	C-N-CA	5.17	134.61	121.70
2	H	127	GLU	CG-CD-OE1	5.15	128.60	118.30
2	H	38	GLN	N-CA-C	-5.14	97.13	111.00
2	H	147	THR	CA-C-N	-5.13	105.91	117.20
2	H	76	TYR	CZ-CE2-CD2	-5.12	115.20	119.80
1	L	14(H)	GLU	CG-CD-OE1	-5.10	108.10	118.30
2	H	129(B)	SER	O-C-N	5.09	130.84	122.70
2	H	197	GLY	CA-C-O	5.08	129.75	120.60
2	H	176	ILE	O-C-N	-5.08	114.58	122.70
2	H	210	MET	CG-SD-CE	-5.07	92.09	100.20
1	L	13	GLU	OE1-CD-OE2	-5.06	117.23	123.30
2	H	135	LYS	C-N-CA	5.05	132.91	122.30
2	H	220	CYS	CA-C-O	-5.04	109.52	120.10
2	H	180	MET	CA-CB-CG	-5.01	104.78	113.30
2	H	145	LYS	CG-CD-CE	5.01	126.93	111.90
1	L	14(D)	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
2	H	53	LEU	CB-CA-C	-5.01	100.68	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	13	GLU	CA-C-O	-5.01	109.59	120.10
2	H	175	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	50	ARG	Sidechain
2	H	97	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	222	0	225	10	0
2	H	2029	0	1993	155	1
3	R	34	0	34	6	0
4	I	78	0	55	9	0
5	H	177	0	0	19	1
5	I	8	0	0	1	0
5	L	20	0	0	2	0
5	R	5	0	0	0	0
All	All	2573	0	2307	169	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (169) 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:79:ILE:HD11	5:H:527:HOH:O	1.16	1.33
4:I:60:PRO:HB2	4:I:62:GLU:OE1	1.43	1.16
2:H:195:SER:HB2	3:R:41:ARG:C	1.64	1.16
2:H:205:ASN:ND2	5:H:483:HOH:O	1.83	1.12
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.39	1.00
2:H:85:LEU:HD13	2:H:106:MET:CE	1.96	0.94
2:H:86:GLU:O	5:H:604:HOH:O	1.85	0.94
2:H:35:ARG:O	2:H:38:GLN:HA	1.70	0.92
2:H:241:VAL:HB	2:H:245:PHE:HE1	1.38	0.89
2:H:83:SER:HB3	5:H:501:HOH:O	1.75	0.86
2:H:50:ARG:HH21	2:H:107:LYS:HE2	1.40	0.85
2:H:73:ARG:HD3	2:H:152:PRO:O	1.79	0.83
2:H:61:GLU:OE2	2:H:87:LYS:HA	1.78	0.81
2:H:221(A):ARG:HG3	5:H:466:HOH:O	1.80	0.79
2:H:17:VAL:O	2:H:188:GLY:HA2	1.82	0.79
2:H:195:SER:HB2	3:R:41:ARG:O	1.83	0.79
2:H:129(B):SER:O	5:H:556:HOH:O	2.06	0.74
2:H:35:ARG:HB2	2:H:39:GLU:HG3	1.71	0.73
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.89	0.72
2:H:62:ASN:C	2:H:64:LEU:H	1.93	0.71
2:H:186(A):ASP:N	2:H:186(A):ASP:OD1	2.24	0.69
2:H:208:TYR:HB3	2:H:210:MET:CE	2.23	0.69
1:L:1(A):ASP:OD1	2:H:119:HIS:HE1	1.74	0.68
2:H:195:SER:CB	3:R:41:ARG:C	2.54	0.67
2:H:62:ASN:HB2	5:H:493:HOH:O	1.93	0.67
2:H:60(I):THR:HG22	2:H:62:ASN:H	1.60	0.67
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.22	0.67
2:H:178:ASP:O	2:H:233:ARG:HD3	1.95	0.66
2:H:85:LEU:CD1	2:H:106:MET:CE	2.72	0.66
2:H:241:VAL:HB	2:H:245:PHE:CE1	2.25	0.65
2:H:208:TYR:HB3	2:H:210:MET:HE1	1.78	0.65
2:H:36(A):SER:HA	2:H:37:PRO:C	2.15	0.65
4:I:60:PRO:HG2	4:I:63:TYS:HE2	1.79	0.64
2:H:137:ARG:HD3	2:H:159:ASN:OD1	1.97	0.63
2:H:126:ARG:NH1	2:H:126:ARG:HG3	2.14	0.63
2:H:35:ARG:O	2:H:38:GLN:CA	2.46	0.62
2:H:60(I):THR:HG22	2:H:62:ASN:HD22	1.64	0.62
2:H:241:VAL:O	2:H:245:PHE:CD1	2.52	0.62
2:H:240:LYS:O	2:H:244:GLN:HB2	1.99	0.62
2:H:219:GLY:CA	2:H:221(A):ARG:HD2	2.22	0.62
2:H:36:LYS:HE2	2:H:62:ASN:O	2.00	0.62
2:H:240:LYS:HE3	2:H:244:GLN:HE22	1.64	0.61
1:L:1(A):ASP:OD1	2:H:119:HIS:CE1	2.54	0.61
2:H:37:PRO:O	2:H:39:GLU:HG2	2.01	0.61
2:H:239:GLN:HG3	5:H:465:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:ARG:CB	2:H:39:GLU:HG3	2.31	0.60
2:H:17:VAL:O	2:H:18:GLU:HB3	2.02	0.60
4:I:57:GLU:HG3	4:I:58:GLU:H	1.66	0.59
2:H:208:TYR:CB	2:H:210:MET:CE	2.81	0.59
2:H:240:LYS:HE3	2:H:244:GLN:NE2	2.18	0.59
2:H:126:ARG:NH1	2:H:126:ARG:CG	2.63	0.59
2:H:74:THR:HG22	2:H:75:ARG:CD	2.33	0.58
2:H:230:HIS:ND1	2:H:233:ARG:HG3	2.18	0.58
2:H:195:SER:CB	3:R:41:ARG:O	2.51	0.58
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.39	0.57
2:H:182:CYS:HA	2:H:226:GLY:O	2.04	0.57
2:H:100:ASP:O	2:H:101:ARG:HB2	2.04	0.57
2:H:23:GLU:OE1	5:H:547:HOH:O	2.17	0.57
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.86	0.57
2:H:126:ARG:HH11	2:H:126:ARG:CG	2.18	0.56
2:H:189:ASP:OD2	3:R:41:ARG:NH2	2.39	0.56
2:H:241:VAL:CB	2:H:245:PHE:HE1	2.13	0.56
2:H:230:HIS:CG	2:H:233:ARG:HG3	2.42	0.55
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.09	0.55
2:H:16:ILE:N	2:H:194:ASP:OD2	2.40	0.55
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.41	0.55
2:H:229:THR:CG2	2:H:234:LEU:HD12	2.37	0.54
2:H:20:SER:O	2:H:157:VAL:N	2.40	0.54
2:H:208:TYR:CB	2:H:210:MET:HE2	2.37	0.54
2:H:57:HIS:HE1	2:H:214:SER:O	1.90	0.54
2:H:221(A):ARG:CG	5:H:466:HOH:O	2.49	0.53
2:H:145:LYS:HD2	5:H:605:HOH:O	2.06	0.53
2:H:217:GLU:O	2:H:221(A):ARG:CD	2.56	0.53
4:I:57:GLU:CG	4:I:58:GLU:N	2.72	0.53
2:H:79:ILE:HD12	2:H:117:TYR:CG	2.44	0.53
2:H:57:HIS:CE1	2:H:195:SER:HG	2.27	0.53
2:H:60(I):THR:CG2	2:H:62:ASN:HD22	2.22	0.53
2:H:134:TYR:HD1	2:H:134:TYR:N	2.06	0.53
2:H:105:LEU:HD13	2:H:241:VAL:CG2	2.39	0.52
2:H:105:LEU:HD13	2:H:241:VAL:HG22	1.92	0.52
2:H:134:TYR:CD1	2:H:134:TYR:N	2.78	0.51
2:H:62:ASN:C	2:H:64:LEU:N	2.62	0.51
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.39	0.51
2:H:208:TYR:HB3	2:H:210:MET:HE2	1.93	0.51
2:H:62:ASN:ND2	2:H:62:ASN:H	2.09	0.51
2:H:64:LEU:HB3	2:H:85:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:LYS:NZ	2:H:80:GLU:OE2	2.45	0.50
2:H:241:VAL:O	2:H:245:PHE:HD1	1.94	0.50
2:H:35:ARG:CB	2:H:39:GLU:CG	2.89	0.49
2:H:178:ASP:O	5:H:429:HOH:O	2.20	0.49
2:H:57:HIS:CD2	2:H:57:HIS:C	2.86	0.49
2:H:60(I):THR:HG22	2:H:62:ASN:ND2	2.26	0.49
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.47	0.49
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	2.12	0.49
2:H:66:VAL:HG11	2:H:108:LEU:HD21	1.93	0.49
2:H:160:LEU:HD22	2:H:184:GLY:HA2	1.95	0.49
4:I:61:GLU:O	4:I:62:GLU:C	2.52	0.49
2:H:70:LYS:HE3	2:H:72:SER:O	2.12	0.49
2:H:40:LEU:C	2:H:40:LEU:HD23	2.33	0.49
2:H:74:THR:HG22	2:H:75:ARG:HD3	1.94	0.48
2:H:50:ARG:HB2	5:H:596:HOH:O	2.13	0.48
2:H:17:VAL:HG23	2:H:191:CYS:HB2	1.96	0.48
2:H:61:GLU:OE2	2:H:88:ILE:N	2.45	0.48
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.11	0.48
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.39	0.48
2:H:17:VAL:O	2:H:18:GLU:CB	2.61	0.48
2:H:208:TYR:CB	2:H:210:MET:HE1	2.43	0.48
2:H:36(A):SER:HA	2:H:38:GLN:N	2.29	0.48
2:H:50:ARG:HH21	2:H:107:LYS:CE	2.20	0.47
2:H:17:VAL:O	2:H:188:GLY:CA	2.58	0.47
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.95	0.47
2:H:217:GLU:O	2:H:221(A):ARG:HD3	2.15	0.47
2:H:35:ARG:HB3	2:H:37:PRO:O	2.15	0.47
2:H:18:GLU:HB3	2:H:188:GLY:HA2	1.96	0.47
1:L:14(E):GLU:OE1	5:L:635:HOH:O	2.20	0.47
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.50	0.47
4:I:56:PHE:HB3	5:I:507:HOH:O	2.16	0.46
1:L:14(A):LYS:NZ	1:L:14(A):LYS:HB2	2.30	0.46
4:I:60:PRO:HG2	4:I:63:TYS:CE2	2.45	0.46
2:H:57:HIS:ND1	2:H:102:ASP:OD2	2.45	0.46
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.51	0.46
2:H:29:TRP:CG	2:H:121:VAL:HB	2.51	0.45
2:H:221(A):ARG:NH1	5:H:580:HOH:O	2.49	0.45
2:H:199:PHE:C	2:H:199:PHE:CD1	2.89	0.45
2:H:147:THR:HA	5:H:620:HOH:O	2.15	0.45
2:H:35:ARG:HB2	2:H:39:GLU:O	2.16	0.45
2:H:76:TYR:CE2	2:H:77(A):ARG:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36(A):SER:CA	2:H:37:PRO:C	2.85	0.45
2:H:136:GLY:O	2:H:159:ASN:HA	2.17	0.44
2:H:85:LEU:HD23	2:H:85:LEU:HA	1.73	0.44
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.98	0.44
2:H:35:ARG:HB3	2:H:39:GLU:HG2	2.00	0.44
2:H:140:GLY:HA3	2:H:194:ASP:OD1	2.16	0.44
2:H:217:GLU:O	2:H:221(A):ARG:HD2	2.17	0.44
4:I:57:GLU:CG	4:I:58:GLU:H	2.31	0.44
2:H:75:ARG:HD3	2:H:75:ARG:N	2.32	0.43
2:H:49:ASP:O	2:H:111:PRO:HA	2.18	0.43
2:H:126:ARG:HG2	2:H:126:ARG:O	2.17	0.43
2:H:165:ARG:N	2:H:166:PRO:HD2	2.33	0.43
2:H:60(G):ASN:O	2:H:60(G):ASN:CG	2.57	0.43
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.54	0.43
2:H:18:GLU:HG3	2:H:18:GLU:O	2.19	0.43
2:H:99:LEU:HD11	3:R:40:PRO:HB3	2.01	0.43
2:H:75:ARG:N	2:H:75:ARG:CD	2.82	0.42
2:H:211:GLY:HA2	2:H:229:THR:O	2.18	0.42
2:H:61:GLU:OE2	2:H:87:LYS:CA	2.58	0.42
2:H:45:SER:O	2:H:52:VAL:HA	2.19	0.42
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.19	0.42
2:H:107:LYS:HB2	2:H:107:LYS:HE3	1.89	0.42
2:H:35:ARG:HB3	2:H:39:GLU:CG	2.49	0.42
4:I:57:GLU:HG3	4:I:58:GLU:N	2.31	0.41
2:H:236:LYS:HB2	5:H:601:HOH:O	2.19	0.41
2:H:60(F):LYS:HE3	5:H:474:HOH:O	2.18	0.41
2:H:242:ILE:C	2:H:244:GLN:H	2.23	0.41
2:H:50:ARG:HD3	5:H:596:HOH:O	2.20	0.41
2:H:60(F):LYS:CD	2:H:60(H):PHE:CE2	3.03	0.41
2:H:131:GLN:O	2:H:132:ALA:C	2.59	0.41
1:L:14(J):TYR:CD1	1:L:14(J):TYR:N	2.85	0.41
2:H:174:ILE:HA	2:H:174:ILE:HD13	1.86	0.41
2:H:245:PHE:N	2:H:245:PHE:CD1	2.88	0.41
2:H:241:VAL:HA	2:H:245:PHE:CE1	2.55	0.41
5:L:504:HOH:O	2:H:135:LYS:HE3	2.19	0.41
1:L:14(G):LEU:HD11	2:H:202:LYS:HG2	2.03	0.41
2:H:163:VAL:HG23	2:H:183:ALA:HA	2.02	0.41
2:H:223:GLY:HA2	5:H:566:HOH:O	2.21	0.40
2:H:233:ARG:HB3	2:H:233:ARG:HE	1.29	0.40
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.56	0.40
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.83	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77(A):ARG:NH1	5:H:564:HOH:O[2_555]	2.02	0.18

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	25/36 (69%)	22 (88%)	3 (12%)	0	100	100
2	H	248/259 (96%)	231 (93%)	17 (7%)	0	100	100
3	R	2/4 (50%)	2 (100%)	0	0	100	100
4	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	282/311 (91%)	262 (93%)	20 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	L	25/31 (81%)	22 (88%)	3 (12%)	6	8
2	H	218/225 (97%)	186 (85%)	32 (15%)	4	4
3	R	4/4 (100%)	4 (100%)	0	100	100
4	I	6/10 (60%)	5 (83%)	1 (17%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	253/270 (94%)	217 (86%)	36 (14%)	4 4

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(A)	ASP
1	L	6	LEU
1	L	14(A)	LYS
2	H	32	MET
2	H	36	LYS
2	H	41	LEU
2	H	50	ARG
2	H	60(E)	ASP
2	H	60(F)	LYS
2	H	62	ASN
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	75	ARG
2	H	79	ILE
2	H	83	SER
2	H	109	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	137	ARG
2	H	147	THR
2	H	154	VAL
2	H	164	GLU
2	H	187	ARG
2	H	192	GLU
2	H	203	SER
2	H	204(B)	ASN
2	H	221(A)	ARG
2	H	233	ARG
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
2	H	243	ASP
2	H	245	PHE
4	I	62	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	62	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN
2	H	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)

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	$\#\|Z\| > 2$
4	TYS	I	63	-	15,16,17	2.14	5 (33%)	16,22,24	3.33	11 (68%)

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
4	TYS	I	63	-	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	63	TYS	OH-CZ	-4.63	1.35	1.42
4	I	63	TYS	O2-S	2.16	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	63	TYS	CB-CA	2.21	1.58	1.53
4	I	63	TYS	O-C	2.75	1.32	1.19
4	I	63	TYS	OH-S	4.14	1.71	1.63

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	63	TYS	O-C-CA	-7.13	106.92	125.49
4	I	63	TYS	CE2-CD2-CG	-3.86	115.76	121.04
4	I	63	TYS	OH-CZ-CE2	-3.69	111.44	118.74
4	I	63	TYS	CB-CG-CD2	-3.23	114.15	120.90
4	I	63	TYS	O3-S-O2	-3.05	97.09	108.56
4	I	63	TYS	CD1-CE1-CZ	-2.45	116.66	119.74
4	I	63	TYS	OH-CZ-CE1	2.26	123.19	118.74
4	I	63	TYS	CE2-CZ-CE1	3.17	125.36	120.20
4	I	63	TYS	O3-S-O1	3.70	122.49	108.56
4	I	63	TYS	CD2-CG-CD1	4.01	124.55	118.13
4	I	63	TYS	O2-S-O1	4.28	131.12	112.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	63	TYS	2	0

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

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.