



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:47 PM GMT

PDB ID : 1HAG
Title : THE ISOMORPHOUS STRUCTURES OF PRETHROMBIN2, HIRUGEN-
AND PPACK-THROMBIN: CHANGES ACCOMPANYING ACTIVATION
AND EXOSITE BINDING TO THROMBIN
Authors : Tulinsky, A.; Vijayalakshmi, J.
Deposited on : 1994-06-27
Resolution : 2.00 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 (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

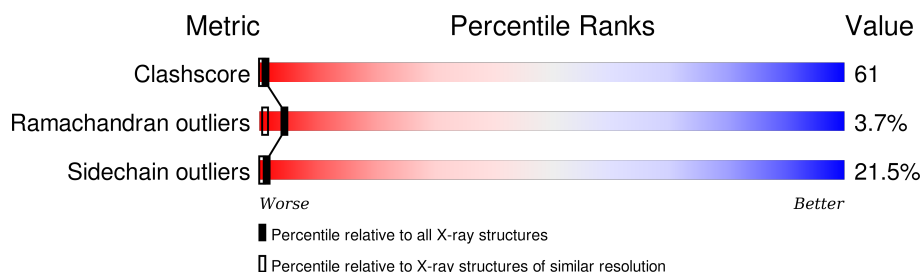
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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	E	295	
2	I	10	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2690 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 PRETHROMBIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	295	Total	C	N	O	S	0	0	0
			2379	1511	418	435	15			

- Molecule 2 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	S	0	0	0
			95	59	10	25	1			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

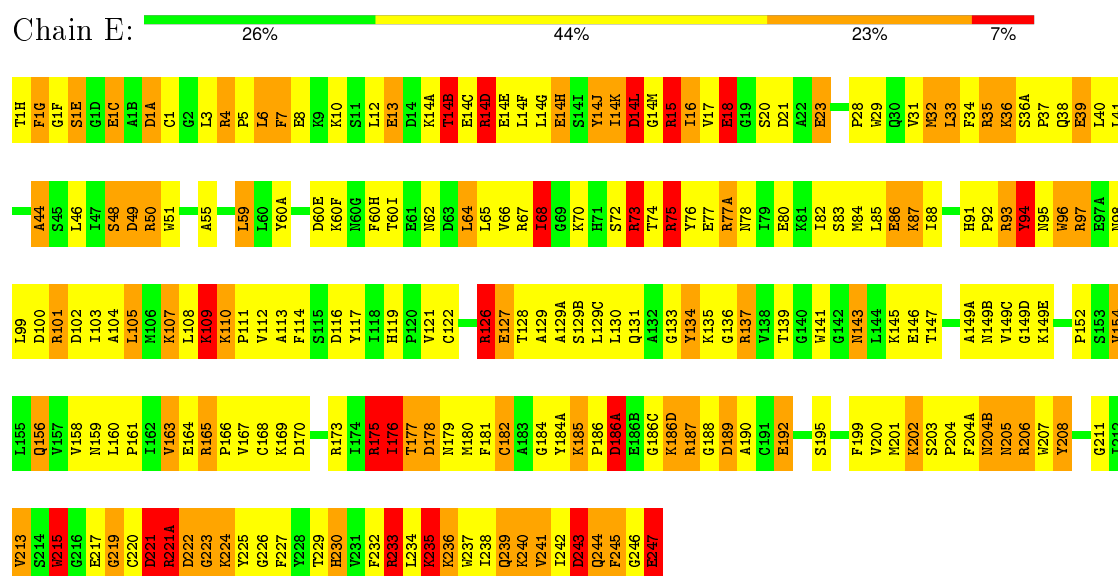
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	188	Total 188	O 188	0	0
4	I	14	Total 14	O 14	0	0

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 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: PRETHROMBIN 2



• Molecule 2: HIRUGEN



4 Data and refinement statistics

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	72.85Å 71.32Å 72.63Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: NAG, 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	E	1.24	2/2438 (0.1%)	2.52	136/3290 (4.1%)
2	I	1.17	0/79	2.43	7/103 (6.8%)
All	All	1.24	2/2517 (0.1%)	2.52	143/3393 (4.2%)

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	E	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	TRP	C-N	-5.13	1.23	1.33
1	E	8	GLU	CD-OE2	-5.02	1.20	1.25

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	ARG	NE-CZ-NH2	21.73	131.16	120.30
1	E	233	ARG	NE-CZ-NH2	19.26	129.93	120.30
1	E	126	ARG	NE-CZ-NH1	-17.69	111.45	120.30
1	E	67	ARG	NE-CZ-NH2	16.29	128.44	120.30
1	E	243	ASP	CB-CG-OD1	15.35	132.11	118.30
1	E	233	ARG	NE-CZ-NH1	-15.22	112.69	120.30
1	E	187	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	E	175	ARG	NE-CZ-NH1	14.13	127.37	120.30
1	E	4	ARG	NE-CZ-NH2	14.09	127.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14(D)	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	E	137	ARG	NE-CZ-NH2	12.62	126.61	120.30
1	E	187	ARG	CD-NE-CZ	12.13	140.59	123.60
1	E	33	LEU	CA-CB-CG	11.94	142.77	115.30
1	E	21	ASP	CB-CG-OD1	11.91	129.02	118.30
1	E	75	ARG	NE-CZ-NH1	-11.81	114.40	120.30
1	E	60(A)	TYR	CB-CG-CD1	-11.68	113.99	121.00
1	E	14(D)	ARG	NE-CZ-NH1	11.65	126.12	120.30
1	E	126	ARG	NE-CZ-NH2	11.33	125.96	120.30
1	E	100	ASP	CB-CG-OD1	10.96	128.16	118.30
1	E	137	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	E	76	TYR	CB-CG-CD2	-10.15	114.91	121.00
1	E	94	TYR	CB-CG-CD2	-10.02	114.99	121.00
1	E	102	ASP	CB-CG-OD1	9.96	127.26	118.30
1	E	129	ALA	CB-CA-C	9.94	125.01	110.10
1	E	1(A)	ASP	CB-CG-OD1	-9.60	109.66	118.30
1	E	60(E)	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	E	206	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	E	21	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	E	126	ARG	CD-NE-CZ	-8.79	111.29	123.60
1	E	186(A)	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	E	60(A)	TYR	CB-CG-CD2	8.72	126.23	121.00
1	E	222	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	E	76	TYR	CB-CG-CD1	8.55	126.13	121.00
1	E	77(A)	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	E	104	ALA	N-CA-CB	8.24	121.63	110.10
1	E	4	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	E	232	PHE	O-C-N	-7.92	110.02	122.70
1	E	186(A)	ASP	CB-CG-OD1	7.85	125.37	118.30
1	E	60(I)	THR	CA-CB-CG2	7.75	123.25	112.40
1	E	80	GLU	CG-CD-OE2	-7.74	102.82	118.30
1	E	13	GLU	CB-CA-C	-7.54	95.32	110.40
1	E	176	ILE	CA-CB-CG2	7.50	125.90	110.90
1	E	101	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	E	67	ARG	NH1-CZ-NH2	-7.27	111.40	119.40
1	E	73	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	E	243	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	E	77	GLU	OE1-CD-OE2	7.12	131.84	123.30
1	E	204(A)	PHE	CB-CG-CD1	-7.01	115.89	120.80
1	E	154	VAL	CA-CB-CG1	7.01	121.42	110.90
1	E	94	TYR	CG-CD1-CE1	-7.00	115.70	121.30
1	E	105	LEU	O-C-N	6.88	133.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	ASN	CA-C-O	-6.87	105.67	120.10
1	E	1(A)	ASP	CA-CB-CG	-6.86	98.31	113.40
1	E	100	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	E	93	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	I	62	GLU	OE1-CD-OE2	6.71	131.36	123.30
1	E	23	GLU	CA-CB-CG	6.69	128.11	113.40
1	E	206	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	E	14(L)	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	E	44	ALA	CB-CA-C	6.56	119.94	110.10
1	E	49	ASP	CB-CG-OD1	6.51	124.16	118.30
1	E	48	SER	CB-CA-C	6.50	122.45	110.10
1	E	3	LEU	CA-CB-CG	6.48	130.21	115.30
1	E	221(A)	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	E	60(I)	THR	CA-CB-OG1	-6.46	95.44	109.00
1	E	187	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	E	117	TYR	C-N-CA	6.38	137.65	121.70
1	E	243	ASP	CA-CB-CG	6.37	127.42	113.40
1	E	97	ARG	CD-NE-CZ	6.30	132.42	123.60
1	E	222	ASP	OD1-CG-OD2	6.29	135.26	123.30
1	E	178	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	E	178	ASP	CB-CG-OD1	6.28	123.95	118.30
2	I	61	GLU	CA-CB-CG	6.25	127.16	113.40
1	E	113	ALA	O-C-N	6.24	132.69	122.70
1	E	247	GLU	CA-C-O	-6.22	107.03	120.10
1	E	18	GLU	OE1-CD-OE2	-6.17	115.90	123.30
2	I	55	ASP	CB-CA-C	6.17	122.74	110.40
1	E	1(E)	SER	C-N-CA	6.16	135.24	122.30
1	E	60(E)	ASP	O-C-N	6.16	132.56	122.70
1	E	175	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	E	14(B)	THR	N-CA-CB	-6.13	98.66	110.30
1	E	240	LYS	CA-C-N	6.08	130.59	117.20
1	E	165	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	E	55	ALA	CB-CA-C	6.07	119.21	110.10
2	I	58	GLU	CG-CD-OE1	6.05	130.41	118.30
1	E	97	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	245	PHE	C-N-CA	6.01	134.91	122.30
1	E	208	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	E	32	MET	O-C-N	5.91	132.16	122.70
1	E	74	THR	N-CA-C	5.90	126.93	111.00
1	E	213	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	E	177	THR	CA-CB-CG2	5.87	120.62	112.40
1	E	181	PHE	CB-CA-C	5.84	122.09	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	ARG	CD-NE-CZ	-5.78	115.50	123.60
1	E	208	TYR	CB-CG-CD1	5.73	124.44	121.00
1	E	200	VAL	CA-CB-CG1	5.70	119.45	110.90
1	E	189	ASP	O-C-N	5.68	131.79	122.70
1	E	68	ILE	CB-CA-C	-5.60	100.40	111.60
1	E	1(C)	GLU	C-N-CA	5.59	135.66	121.70
1	E	75	ARG	CG-CD-NE	5.57	123.49	111.80
1	E	8	GLU	O-C-N	5.54	131.56	122.70
1	E	134	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	E	190	ALA	O-C-N	5.51	131.52	122.70
1	E	232	PHE	CA-C-N	5.50	129.30	117.20
1	E	202	LYS	CB-CA-C	-5.49	99.41	110.40
1	E	240	LYS	CA-C-O	-5.47	108.61	120.10
1	E	224	LYS	CB-CA-C	5.45	121.31	110.40
1	E	201	MET	CG-SD-CE	5.39	108.83	100.20
1	E	14(L)	ASP	CB-CA-C	5.39	121.17	110.40
1	E	80	GLU	CG-CD-OE1	5.38	129.06	118.30
1	E	18	GLU	CB-CG-CD	5.36	128.68	114.20
1	E	164	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	E	3	LEU	CB-CA-C	5.33	120.32	110.20
1	E	208	TYR	CA-CB-CG	5.32	123.51	113.40
1	E	60(I)	THR	N-CA-CB	-5.32	100.20	110.30
2	I	64	LEU	CB-CA-C	5.31	120.30	110.20
1	E	76	TYR	CB-CA-C	5.30	121.00	110.40
1	E	7	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	E	78	ASN	CB-CG-ND2	5.28	129.37	116.70
1	E	102	ASP	CA-CB-CG	5.26	124.97	113.40
1	E	96	TRP	CB-CA-C	5.22	120.85	110.40
1	E	225	TYR	N-CA-CB	-5.22	101.21	110.60
1	E	109	LYS	CA-CB-CG	5.20	124.85	113.40
1	E	186(A)	ASP	CA-CB-CG	5.20	124.84	113.40
2	I	64	LEU	CA-CB-CG	-5.19	103.36	115.30
1	E	39	GLU	CG-CD-OE1	-5.18	107.93	118.30
1	E	14(L)	ASP	C-N-CA	-5.18	111.42	122.30
1	E	184	GLY	O-C-N	5.18	130.98	122.70
1	E	23	GLU	N-CA-CB	5.17	119.91	110.60
1	E	163	VAL	CA-CB-CG1	5.16	118.64	110.90
1	E	75	ARG	CB-CG-CD	5.14	124.96	111.60
1	E	8	GLU	OE1-CD-OE2	5.14	129.47	123.30
2	I	64	LEU	N-CA-CB	-5.14	100.12	110.40
1	E	163	VAL	CB-CA-C	5.12	121.12	111.40
1	E	1(C)	GLU	CA-CB-CG	5.11	124.65	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	101	ARG	CD-NE-CZ	-5.11	116.44	123.60
1	E	86	GLU	CG-CD-OE1	-5.07	108.17	118.30
1	E	205	ASN	CA-CB-CG	-5.06	102.27	113.40
1	E	13	GLU	CA-CB-CG	5.06	124.53	113.40
1	E	235	LYS	O-C-N	5.06	130.79	122.70
1	E	170	ASP	CB-CG-OD1	5.04	122.83	118.30
1	E	145	LYS	C-N-CA	5.03	134.27	121.70
1	E	80	GLU	CA-CB-CG	5.01	124.41	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	126	ARG	Sidechain
1	E	14(D)	ARG	Sidechain
1	E	15	ARG	Sidechain
1	E	175	ARG	Sidechain
1	E	73	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2379	0	2342	293	0
2	I	95	0	72	6	0
3	E	14	0	13	2	0
4	E	188	0	0	32	0
4	I	14	0	0	0	0
All	All	2690	0	2427	298	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 61.

All (298) 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:E:185:LYS:HE2	1:E:186(D):LYS:CE	1.63	1.28
1:E:14(K):ILE:CD1	1:E:161:PRO:HB3	1.62	1.27
1:E:188:GLY:HA2	4:E:521:HOH:O	1.34	1.23
1:E:75:ARG:CA	1:E:75:ARG:NH1	2.01	1.23
1:E:75:ARG:CB	1:E:75:ARG:HH11	1.59	1.15
1:E:75:ARG:NH1	1:E:75:ARG:HA	1.60	1.14
1:E:75:ARG:CA	1:E:75:ARG:HH11	1.58	1.13
1:E:14(K):ILE:HD11	1:E:161:PRO:HB3	1.13	1.13
1:E:185:LYS:CE	1:E:186(D):LYS:HE2	1.80	1.11
1:E:186:PRO:CB	1:E:223:GLY:HA3	1.80	1.10
1:E:14(D):ARG:H	1:E:14(D):ARG:HD2	0.97	1.07
1:E:110:LYS:HG3	1:E:111:PRO:HD2	1.36	1.06
1:E:245:PHE:O	4:E:556:HOH:O	1.72	1.06
1:E:186:PRO:HB3	1:E:223:GLY:HA3	1.09	1.05
1:E:185:LYS:HE2	1:E:186(D):LYS:HE2	1.05	1.05
1:E:35:ARG:HG3	1:E:41:LEU:HD11	1.38	1.03
1:E:186:PRO:HB3	1:E:223:GLY:CA	1.87	1.02
1:E:109:LYS:HE2	4:E:520:HOH:O	1.57	1.02
1:E:14(C):GLU:O	1:E:14(G):LEU:HD23	1.59	1.01
1:E:75:ARG:HH11	1:E:75:ARG:CG	1.63	0.99
1:E:149(E):LYS:O	1:E:149(E):LYS:HG2	1.56	0.99
1:E:18:GLU:HB3	1:E:187:ARG:HE	1.25	0.98
1:E:75:ARG:HA	1:E:75:ARG:HH12	1.18	0.97
1:E:130:LEU:CD1	1:E:230:HIS:CE1	2.47	0.97
1:E:14(D):ARG:HD2	1:E:14(D):ARG:N	1.76	0.95
1:E:185:LYS:HE2	1:E:186(D):LYS:NZ	1.83	0.93
1:E:49:ASP:O	1:E:112:VAL:HG12	1.67	0.93
1:E:204(B):ASN:C	1:E:204(B):ASN:HD22	1.67	0.92
1:E:14(B):THR:HG23	1:E:159:ASN:HD21	1.32	0.92
1:E:221:ASP:OD2	4:E:460:HOH:O	1.86	0.91
1:E:16:ILE:HD11	1:E:187:ARG:N	1.86	0.90
1:E:14(K):ILE:HD11	1:E:161:PRO:CB	1.99	0.90
1:E:186:PRO:HG3	1:E:223:GLY:O	1.73	0.88
1:E:14(B):THR:HG22	1:E:137:ARG:NH2	1.90	0.87
1:E:186:PRO:HG3	1:E:223:GLY:C	1.96	0.85
1:E:14(J):TYR:HD1	1:E:14(J):TYR:H	1.23	0.85
1:E:186(C):GLY:O	1:E:186(D):LYS:HE3	1.76	0.85
1:E:186(A):ASP:HB3	1:E:186(D):LYS:NZ	1.90	0.85
1:E:222:ASP:O	1:E:224:LYS:HG3	1.77	0.85
1:E:128:THR:HG22	1:E:129(C):LEU:HD12	1.57	0.84
1:E:14(D):ARG:H	1:E:14(D):ARG:CD	1.87	0.84
1:E:73:ARG:HG3	1:E:141:TRP:CD1	2.12	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LYS:CG	1:E:111:PRO:HD2	2.07	0.83
1:E:72:SER:OG	1:E:75:ARG:HG3	1.78	0.83
1:E:241:VAL:O	1:E:245:PHE:HB2	1.78	0.82
1:E:14(B):THR:HG22	1:E:137:ARG:HH21	1.44	0.82
1:E:14(A):LYS:HD3	4:E:585:HOH:O	1.78	0.81
1:E:98:ASN:O	1:E:99:LEU:HB2	1.80	0.81
1:E:103:ILE:HG21	1:E:234:LEU:HD13	1.61	0.81
1:E:186(A):ASP:HB3	1:E:186(D):LYS:HZ2	1.47	0.80
1:E:130:LEU:HD11	1:E:230:HIS:CE1	2.15	0.80
1:E:192:GLU:OE2	4:E:474:HOH:O	1.98	0.79
1:E:188:GLY:CA	4:E:521:HOH:O	2.06	0.79
1:E:35:ARG:HG3	1:E:41:LEU:CD1	2.10	0.79
1:E:1(H):THR:O	1:E:1(H):THR:HG23	1.82	0.79
1:E:130:LEU:HD12	1:E:230:HIS:CE1	2.16	0.79
1:E:16:ILE:HD11	1:E:186(D):LYS:HA	1.63	0.78
1:E:186(A):ASP:CB	1:E:186(D):LYS:HD3	2.14	0.78
1:E:75:ARG:N	1:E:75:ARG:NH1	2.32	0.78
1:E:130:LEU:HD12	1:E:230:HIS:HE1	1.48	0.77
1:E:16:ILE:HD11	1:E:186(D):LYS:CA	2.13	0.77
1:E:204(B):ASN:C	1:E:204(B):ASN:ND2	2.36	0.77
1:E:14(K):ILE:CD1	1:E:161:PRO:CB	2.56	0.77
1:E:189:ASP:O	1:E:192:GLU:HB2	1.83	0.77
1:E:128:THR:CG2	1:E:129(C):LEU:HD12	2.15	0.76
1:E:219:GLY:N	1:E:224:LYS:HE3	2.00	0.76
1:E:16:ILE:HD11	1:E:187:ARG:H	1.47	0.76
1:E:147:THR:OG1	1:E:149(A):ALA:HB3	1.86	0.76
1:E:35:ARG:CG	1:E:41:LEU:HD11	2.15	0.76
1:E:127:GLU:OE2	4:E:489:HOH:O	2.04	0.75
1:E:72:SER:OG	1:E:75:ARG:CG	2.35	0.74
1:E:239:GLN:HG3	4:E:436:HOH:O	1.85	0.74
1:E:109:LYS:NZ	4:E:508:HOH:O	2.22	0.72
1:E:97:ARG:HG3	4:E:419:HOH:O	1.89	0.72
1:E:36:LYS:O	1:E:38:GLN:HG3	1.89	0.71
1:E:103:ILE:CG2	1:E:234:LEU:HD13	2.21	0.71
1:E:185:LYS:HE2	1:E:186(D):LYS:HZ3	1.56	0.71
1:E:64:LEU:O	4:E:449:HOH:O	2.09	0.71
1:E:204(B):ASN:HD22	1:E:205:ASN:N	1.87	0.71
1:E:49:ASP:HB3	1:E:114:PHE:CZ	2.26	0.71
1:E:14(K):ILE:HD12	1:E:161:PRO:HB3	1.71	0.70
1:E:94:TYR:HB2	1:E:101:ARG:O	1.92	0.70
1:E:185:LYS:CD	1:E:186(D):LYS:HE2	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LEU:HD22	1:E:88:ILE:HD13	1.73	0.70
1:E:75:ARG:CB	1:E:75:ARG:NH1	2.39	0.69
1:E:75:ARG:NH1	1:E:75:ARG:CG	2.41	0.69
1:E:110:LYS:HG3	1:E:111:PRO:CD	2.19	0.69
1:E:18:GLU:HB3	1:E:187:ARG:NE	2.04	0.68
1:E:93:ARG:NH1	4:E:539:HOH:O	2.27	0.68
1:E:35:ARG:CG	1:E:41:LEU:CD1	2.72	0.67
1:E:32:MET:CG	1:E:40:LEU:HD13	2.25	0.67
1:E:35:ARG:O	1:E:38:GLN:HA	1.94	0.67
1:E:84:MET:O	1:E:109:LYS:HB2	1.94	0.67
1:E:18:GLU:HA	1:E:187:ARG:HB3	1.75	0.67
1:E:73:ARG:HG3	1:E:141:TRP:CG	2.30	0.67
1:E:14(E):GLU:O	1:E:14(H):GLU:HG3	1.94	0.66
1:E:59:LEU:HD13	1:E:88:ILE:HG21	1.75	0.66
1:E:147:THR:HG21	1:E:149(A):ALA:HB2	1.77	0.66
1:E:188:GLY:N	4:E:521:HOH:O	2.26	0.66
1:E:1(G):PHE:HD1	1:E:1(G):PHE:O	1.79	0.66
1:E:109:LYS:HD2	4:E:508:HOH:O	1.95	0.65
1:E:16:ILE:CD1	1:E:187:ARG:H	2.08	0.65
1:E:185:LYS:HD3	1:E:185:LYS:N	2.12	0.65
1:E:185:LYS:O	1:E:186(D):LYS:CG	2.44	0.65
1:E:14(D):ARG:O	1:E:14(G):LEU:HB2	1.96	0.65
1:E:5:PRO:HG3	4:E:523:HOH:O	1.96	0.65
1:E:175:ARG:HB3	4:E:410:HOH:O	1.96	0.64
1:E:126:ARG:HG3	1:E:126:ARG:O	1.96	0.64
1:E:186(A):ASP:HB3	1:E:186(D):LYS:HD3	1.78	0.64
1:E:185:LYS:O	1:E:186(D):LYS:HG2	1.97	0.64
1:E:215:TRP:CZ3	1:E:227:PHE:CG	2.85	0.64
1:E:129(A):ALA:O	4:E:602:HOH:O	2.15	0.64
1:E:235:LYS:HA	1:E:238:ILE:HD12	1.78	0.64
1:E:244:GLN:C	1:E:244:GLN:OE1	2.36	0.64
1:E:203:SER:HB3	1:E:204(B):ASN:ND2	2.13	0.63
1:E:203:SER:HB3	1:E:204(B):ASN:HD21	1.63	0.63
1:E:143:ASN:O	1:E:146:GLU:HG3	1.98	0.63
1:E:223:GLY:C	1:E:224:LYS:HG2	2.19	0.63
1:E:1(G):PHE:O	1:E:1(E):SER:N	2.31	0.63
1:E:16:ILE:HD11	1:E:186(D):LYS:C	2.19	0.63
1:E:85:LEU:HD12	4:E:449:HOH:O	1.98	0.62
1:E:35:ARG:HB2	1:E:41:LEU:CD1	2.29	0.62
1:E:219:GLY:H	1:E:224:LYS:HE3	1.63	0.62
1:E:4:ARG:HG2	1:E:28:PRO:CG	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:LEU:HD22	1:E:64:LEU:CD2	2.29	0.62
1:E:217:GLU:HB3	1:E:224:LYS:HB3	1.82	0.62
1:E:186:PRO:CG	1:E:223:GLY:O	2.48	0.61
1:E:91:HIS:ND1	1:E:92:PRO:HD2	2.15	0.61
1:E:158:VAL:HG21	1:E:188:GLY:HA2	1.82	0.61
1:E:224:LYS:HE2	4:E:497:HOH:O	2.00	0.61
1:E:75:ARG:N	1:E:75:ARG:HH11	1.95	0.61
1:E:14(B):THR:CG2	1:E:137:ARG:HH21	2.11	0.61
1:E:185:LYS:N	1:E:185:LYS:CD	2.60	0.60
1:E:186:PRO:CG	1:E:223:GLY:HA3	2.31	0.60
1:E:41:LEU:HD21	1:E:60(H):PHE:CE2	2.36	0.60
1:E:149(E):LYS:O	1:E:149(E):LYS:CG	2.37	0.60
1:E:14(J):TYR:CD1	1:E:14(J):TYR:N	2.70	0.60
1:E:185:LYS:H	1:E:185:LYS:CD	1.97	0.60
1:E:235:LYS:O	1:E:235:LYS:HG2	2.00	0.60
3:E:400:NAG:H4	4:E:560:HOH:O	2.02	0.60
1:E:75:ARG:HH11	1:E:75:ARG:HG2	1.63	0.59
1:E:14(F):LEU:HB3	4:E:406:HOH:O	2.03	0.59
1:E:186(A):ASP:CB	1:E:186(D):LYS:NZ	2.64	0.58
1:E:165:ARG:HH22	1:E:177:THR:C	2.07	0.58
1:E:186(D):LYS:N	1:E:186(D):LYS:HD2	2.19	0.58
1:E:84:MET:CE	2:I:63:TYS:O	2.52	0.58
1:E:32:MET:HG2	1:E:40:LEU:HD13	1.86	0.58
1:E:10:LYS:NZ	4:E:486:HOH:O	2.37	0.57
1:E:211:GLY:HA2	1:E:229:THR:O	2.04	0.57
1:E:176:ILE:HD12	1:E:180:MET:HB2	1.85	0.57
1:E:203:SER:HB2	1:E:208:TYR:HE1	1.70	0.57
1:E:41:LEU:HD22	1:E:64:LEU:HD22	1.86	0.56
1:E:247:GLU:O	1:E:247:GLU:HG3	2.04	0.56
1:E:70:LYS:HE3	1:E:72:SER:O	2.05	0.56
1:E:1(H):THR:CG2	1:E:1(H):THR:O	2.51	0.56
1:E:217:GLU:CB	1:E:224:LYS:HB3	2.35	0.56
1:E:16:ILE:CD1	1:E:186(D):LYS:HA	2.33	0.56
1:E:35:ARG:HB3	1:E:39:GLU:HG2	1.88	0.56
1:E:186(C):GLY:C	1:E:186(D):LYS:HD2	2.27	0.55
1:E:215:TRP:CZ3	1:E:227:PHE:CD1	2.95	0.55
1:E:66:VAL:HG21	1:E:108:LEU:HD21	1.89	0.55
1:E:16:ILE:CD1	1:E:187:ARG:N	2.65	0.55
2:I:59:ILE:HG13	2:I:59:ILE:O	2.05	0.55
1:E:217:GLU:HB3	1:E:224:LYS:CB	2.36	0.55
1:E:185:LYS:CE	1:E:186(D):LYS:CE	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14(G):LEU:N	1:E:14(G):LEU:HD22	2.22	0.54
1:E:135:LYS:HE2	1:E:184(A):TYR:OH	2.08	0.54
1:E:105:LEU:HD12	1:E:241:VAL:CG1	2.38	0.54
1:E:49:ASP:HB3	1:E:114:PHE:HZ	1.67	0.54
1:E:203:SER:N	1:E:206:ARG:O	2.38	0.54
1:E:182:CYS:HA	1:E:226:GLY:O	2.08	0.54
1:E:14(M):GLY:O	1:E:15:ARG:C	2.47	0.54
1:E:219:GLY:O	1:E:221:ASP:N	2.40	0.53
1:E:14(F):LEU:N	1:E:14(F):LEU:HD12	2.22	0.53
1:E:14(F):LEU:CD1	1:E:14(F):LEU:N	2.70	0.53
1:E:136:GLY:HA3	1:E:199:PHE:CZ	2.44	0.53
1:E:158:VAL:HG21	1:E:188:GLY:CA	2.39	0.53
1:E:49:ASP:CB	1:E:114:PHE:CZ	2.92	0.53
1:E:86:GLU:O	1:E:87:LYS:HG2	2.09	0.52
1:E:234:LEU:O	1:E:237:TRP:HB3	2.09	0.52
3:E:400:NAG:C4	4:E:560:HOH:O	2.57	0.52
1:E:186:PRO:HG3	1:E:223:GLY:CA	2.40	0.52
1:E:239:GLN:HA	4:E:436:HOH:O	2.08	0.52
1:E:35:ARG:CB	1:E:39:GLU:HG2	2.40	0.52
1:E:236:LYS:O	1:E:240:LYS:HG2	2.10	0.51
1:E:221:ASP:CG	1:E:221(A):ARG:N	2.64	0.51
1:E:14(K):ILE:O	1:E:14(L):ASP:C	2.49	0.51
1:E:84:MET:HE3	2:I:63:TYS:O	2.11	0.51
1:E:241:VAL:O	1:E:245:PHE:CB	2.56	0.51
1:E:35:ARG:CB	1:E:41:LEU:CD1	2.88	0.51
1:E:59:LEU:HD22	1:E:88:ILE:CD1	2.38	0.51
1:E:17:VAL:O	1:E:17:VAL:HG13	2.10	0.51
1:E:186(A):ASP:CA	1:E:186(D):LYS:HD3	2.40	0.51
1:E:51:TRP:CZ3	1:E:107:LYS:HB3	2.45	0.51
1:E:7:PHE:O	1:E:12:LEU:N	2.39	0.51
1:E:35:ARG:HB2	1:E:41:LEU:HD12	1.94	0.50
1:E:49:ASP:C	1:E:112:VAL:HG12	2.31	0.50
1:E:163:VAL:HG12	1:E:168:CYS:SG	2.50	0.50
1:E:29:TRP:CG	1:E:121:VAL:HB	2.46	0.50
1:E:5:PRO:HB3	4:E:555:HOH:O	2.10	0.50
1:E:204(B):ASN:ND2	1:E:206:ARG:H	2.10	0.50
1:E:139:THR:HA	1:E:156:GLN:O	2.12	0.50
1:E:217:GLU:CB	1:E:224:LYS:CB	2.90	0.50
1:E:14(K):ILE:HB	1:E:133:GLY:O	2.12	0.49
1:E:165:ARG:NH2	1:E:178:ASP:HA	2.27	0.49
1:E:18:GLU:CA	1:E:187:ARG:HB3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:CYS:O	1:E:208:TYR:HA	2.11	0.49
1:E:36(A):SER:HA	1:E:37:PRO:C	2.32	0.49
1:E:242:ILE:HG22	1:E:243:ASP:N	2.26	0.49
1:E:202:LYS:HE3	1:E:205:ASN:O	2.12	0.49
1:E:186(C):GLY:O	1:E:186(D):LYS:CE	2.56	0.49
1:E:14(D):ARG:O	1:E:14(G):LEU:N	2.46	0.49
1:E:14(H):GLU:HB2	1:E:14(J):TYR:O	2.12	0.49
1:E:135:LYS:HE2	1:E:184(A):TYR:CZ	2.48	0.49
1:E:66:VAL:HG21	1:E:108:LEU:CD2	2.42	0.49
1:E:185:LYS:CE	1:E:186(D):LYS:HZ3	2.25	0.48
1:E:186(A):ASP:CB	1:E:186(D):LYS:HZ3	2.26	0.48
1:E:186(A):ASP:HB3	1:E:186(D):LYS:CD	2.43	0.48
1:E:72:SER:OG	1:E:75:ARG:HG2	2.12	0.48
1:E:32:MET:HG3	1:E:40:LEU:HD13	1.95	0.48
1:E:14(J):TYR:HD1	1:E:14(J):TYR:N	1.99	0.47
1:E:91:HIS:CE1	1:E:93:ARG:HB2	2.48	0.47
1:E:235:LYS:O	1:E:235:LYS:CG	2.62	0.47
1:E:16:ILE:O	1:E:16:ILE:HG12	2.15	0.47
1:E:185:LYS:CE	1:E:186(D):LYS:NZ	2.67	0.47
1:E:1(C):GLU:HG3	1:E:1:CYS:HB3	1.97	0.47
1:E:84:MET:HE2	2:I:63:TYS:O	2.15	0.47
1:E:105:LEU:HD12	1:E:241:VAL:HG11	1.96	0.47
1:E:143:ASN:C	1:E:143:ASN:OD1	2.53	0.46
1:E:186:PRO:CG	1:E:223:GLY:CA	2.94	0.46
1:E:14(G):LEU:CD2	1:E:14(G):LEU:N	2.77	0.46
1:E:173:ARG:HB3	4:E:557:HOH:O	2.14	0.46
1:E:221:ASP:CG	1:E:221(A):ARG:H	2.20	0.45
1:E:163:VAL:CG1	1:E:182:CYS:SG	3.04	0.45
1:E:135:LYS:HA	1:E:160:LEU:O	2.17	0.45
1:E:107:LYS:CD	1:E:246:GLY:HA2	2.47	0.45
1:E:185:LYS:HD3	1:E:186(D):LYS:HE2	1.97	0.45
1:E:14(D):ARG:HH11	1:E:14(D):ARG:N	2.14	0.45
1:E:129(C):LEU:HD21	1:E:204:PRO:HD3	1.99	0.44
1:E:14(A):LYS:CE	4:E:585:HOH:O	2.64	0.44
1:E:221:ASP:OD1	1:E:221(A):ARG:N	2.50	0.44
1:E:6:LEU:HD11	1:E:116:ASP:CG	2.38	0.44
1:E:75:ARG:H	1:E:75:ARG:HG2	1.32	0.44
1:E:73:ARG:HD3	1:E:152:PRO:O	2.17	0.44
1:E:91:HIS:NE2	1:E:101:ARG:HD2	2.33	0.44
1:E:217:GLU:C	1:E:224:LYS:HB2	2.37	0.44
2:I:60:PRO:HB2	2:I:62:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1(G):PHE:CD1	1:E:1(G):PHE:O	2.65	0.44
1:E:31:VAL:HG22	1:E:68:ILE:HD13	2.00	0.44
1:E:203:SER:HB2	1:E:208:TYR:CE1	2.52	0.43
1:E:165:ARG:HB3	1:E:166:PRO:HD3	2.00	0.43
1:E:50:ARG:HE	1:E:50:ARG:HB2	1.14	0.43
1:E:186(A):ASP:HB2	1:E:186(D):LYS:HD3	1.99	0.43
1:E:14(F):LEU:CD1	1:E:14(F):LEU:H	2.31	0.43
1:E:129(A):ALA:HA	4:E:493:HOH:O	2.19	0.43
1:E:49:ASP:O	1:E:112:VAL:N	2.50	0.43
1:E:95:ASN:O	1:E:99:LEU:N	2.49	0.43
1:E:29:TRP:CD2	1:E:121:VAL:HB	2.54	0.43
2:I:60:PRO:C	2:I:62:GLU:N	2.72	0.43
1:E:86:GLU:OE1	1:E:107:LYS:HD3	2.19	0.42
1:E:14(F):LEU:HD22	1:E:207:TRP:HH2	1.83	0.42
1:E:130:LEU:O	1:E:131:GLN:HG3	2.19	0.42
1:E:91:HIS:CG	1:E:92:PRO:HD2	2.53	0.42
1:E:17:VAL:O	1:E:17:VAL:CG1	2.67	0.42
1:E:185:LYS:O	1:E:186:PRO:C	2.57	0.42
1:E:107:LYS:HD2	1:E:246:GLY:HA2	2.02	0.42
1:E:217:GLU:HA	1:E:217:GLU:OE1	2.20	0.42
1:E:175:ARG:NE	4:E:522:HOH:O	2.53	0.42
1:E:163:VAL:HB	1:E:182:CYS:SG	2.60	0.42
1:E:221(A):ARG:HA	1:E:221(A):ARG:HD2	1.92	0.42
1:E:66:VAL:O	1:E:82:ILE:HA	2.20	0.42
1:E:134:TYR:N	1:E:134:TYR:HD1	2.17	0.42
1:E:34:PHE:CE2	1:E:38:GLN:HG2	2.55	0.41
1:E:242:ILE:C	1:E:244:GLN:N	2.73	0.41
1:E:165:ARG:O	1:E:169:LYS:HG3	2.20	0.41
1:E:94:TYR:HE1	1:E:99:LEU:HD22	1.86	0.41
1:E:235:LYS:O	1:E:239:GLN:HB2	2.20	0.41
1:E:1(G):PHE:C	1:E:1(E):SER:N	2.74	0.41
1:E:242:ILE:C	1:E:244:GLN:H	2.24	0.41
1:E:6:LEU:N	1:E:6:LEU:CD1	2.83	0.41
1:E:230:HIS:CD2	1:E:233:ARG:CG	3.03	0.41
1:E:237:TRP:HB2	4:E:427:HOH:O	2.19	0.41
1:E:14(E):GLU:OE2	1:E:135:LYS:HD2	2.20	0.41
1:E:103:ILE:HG21	1:E:234:LEU:CD1	2.43	0.41
1:E:236:LYS:HD3	1:E:239:GLN:HB3	2.01	0.41
1:E:14(C):GLU:HG3	1:E:14(D):ARG:NH1	2.36	0.41
1:E:1(G):PHE:HE1	1:E:243:ASP:HA	1.86	0.41
1:E:149(B):ASN:O	1:E:149(D):GLY:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:VAL:O	1:E:167:VAL:CG1	2.69	0.41
1:E:105:LEU:HD12	1:E:241:VAL:HG13	2.02	0.40
1:E:128:THR:CG2	1:E:129(C):LEU:CD1	2.95	0.40
1:E:96:TRP:O	1:E:97:ARG:C	2.59	0.40
1:E:28:PRO:HB2	1:E:119:HIS:HB3	2.04	0.40
1:E:33:LEU:HD21	1:E:44:ALA:HB2	2.03	0.40
1:E:222:ASP:O	1:E:224:LYS:CG	2.61	0.40
1:E:14(K):ILE:HG21	1:E:14(K):ILE:HD13	1.62	0.40
1:E:1(G):PHE:C	1:E:1(E):SER:H	2.25	0.40
1:E:163:VAL:O	4:E:435:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	E	293/295 (99%)	247 (84%)	35 (12%)	11 (4%)	4	1
2	I	7/10 (70%)	4 (57%)	3 (43%)	0	100	100
All	All	300/305 (98%)	251 (84%)	38 (13%)	11 (4%)	4	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1(F)	GLY
1	E	149(C)	VAL
1	E	223	GLY
1	E	18	GLU
1	E	243	ASP
1	E	15	ARG
1	E	20	SER
1	E	221	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	221(A)	ARG
1	E	219	GLY
1	E	213	VAL

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	E	256/256 (100%)	200 (78%)	56 (22%)	1	0
2	I	9/9 (100%)	8 (89%)	1 (11%)	8	4
All	All	265/265 (100%)	208 (78%)	57 (22%)	1	0

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1(G)	PHE
1	E	1(A)	ASP
1	E	6	LEU
1	E	13	GLU
1	E	14(B)	THR
1	E	14(D)	ARG
1	E	14(H)	GLU
1	E	14(J)	TYR
1	E	14(K)	ILE
1	E	14(L)	ASP
1	E	16	ILE
1	E	23	GLU
1	E	35	ARG
1	E	36	LYS
1	E	46	LEU
1	E	48	SER
1	E	50	ARG
1	E	59	LEU
1	E	60(F)	LYS
1	E	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	64	LEU
1	E	65	LEU
1	E	68	ILE
1	E	75	ARG
1	E	77(A)	ARG
1	E	83	SER
1	E	87	LYS
1	E	94	TYR
1	E	107	LYS
1	E	109	LYS
1	E	110	LYS
1	E	127	GLU
1	E	129(B)	SER
1	E	143	ASN
1	E	154	VAL
1	E	156	GLN
1	E	175	ARG
1	E	176	ILE
1	E	182	CYS
1	E	185	LYS
1	E	186(A)	ASP
1	E	186(D)	LYS
1	E	192	GLU
1	E	195	SER
1	E	204(B)	ASN
1	E	215	TRP
1	E	220	CYS
1	E	221	ASP
1	E	230	HIS
1	E	233	ARG
1	E	235	LYS
1	E	236	LYS
1	E	239	GLN
1	E	241	VAL
1	E	244	GLN
1	E	247	GLU
2	I	62	GLU

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

Mol	Chain	Res	Type
1	E	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	156	GLN
1	E	159	ASN
1	E	204(B)	ASN
1	E	230	HIS

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$
2	TYS	I	63	2	15,16,17	1.70	3 (20%)	16,22,24	2.40	8 (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
2	TYS	I	63	2	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	63	TYS	OH-CZ	-4.87	1.34	1.42
2	I	63	TYS	O3-S	-2.06	1.39	1.50
2	I	63	TYS	O1-S	2.06	1.52	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	63	TYS	CG-CB-CA	-3.36	106.61	114.21
2	I	63	TYS	O-C-CA	-2.35	119.37	125.49
2	I	63	TYS	CE1-CD1-CG	-2.25	117.96	121.04
2	I	63	TYS	O2-S-O1	-2.15	103.10	112.46
2	I	63	TYS	CD2-CG-CD1	2.09	121.48	118.13
2	I	63	TYS	OH-CZ-CE1	2.16	123.00	118.74
2	I	63	TYS	O3-S-O2	2.36	117.42	108.56
2	I	63	TYS	CZ-OH-S	6.42	129.45	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	63	TYS	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	NAG	E	400	1	14,14,15	0.65	0	15,19,21	1.50	4 (26%)

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	NAG	E	400	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	400	NAG	C2-N2-C7	-2.65	119.64	123.04
3	E	400	NAG	O6-C6-C5	-2.51	103.04	111.33
3	E	400	NAG	C3-C4-C5	-2.04	106.65	110.20
3	E	400	NAG	O7-C7-C8	2.42	126.50	122.06

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
3	E	400	NAG	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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