Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BKC
Title	:	CATALYTIC DOMAIN OF TNF-ALPHA CONVERTING ENZYME (TACE)
Authors	:	Maskos, K.; Fernandez-Catalan, C.; Bode, W.
Deposited on	:	1998-04-23
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 (i) symbol.

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

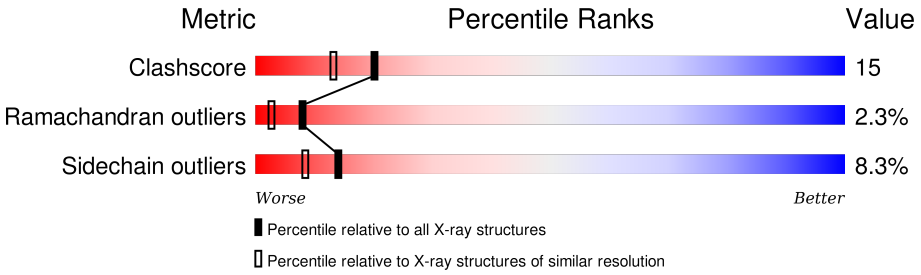
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	68% 25% 5%
1	C	256	63% 25% 9%
2	E	256	69% 26%
3	I	256	71% 22% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	INN	A	2	X	-	-	-
5	INN	C	2	X	-	-	-
5	INN	E	2	X	-	-	-
5	INN	I	2	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9822 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 TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	9	0	0
			2025	1274	342	396	13			
1	C	254	Total	C	N	O	S	127	0	0
			2012	1265	340	394	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	ENGINEERED	UNP P78536
A	452	GLN	ASN	ENGINEERED	UNP P78536
C	266	ALA	SER	ENGINEERED	UNP P78536
C	452	GLN	ASN	ENGINEERED	UNP P78536

- Molecule 2 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	256	Total	C	N	O	S	18	0	0
			2028	1275	344	396	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	266	ALA	SER	ENGINEERED	UNP P78536
E	420	LYS	LEU	CONFLICT	UNP P78536
E	452	GLN	ASN	ENGINEERED	UNP P78536

- Molecule 3 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	254	Total	C	N	O	S	48	0	0
			2017	1269	341	394	13			

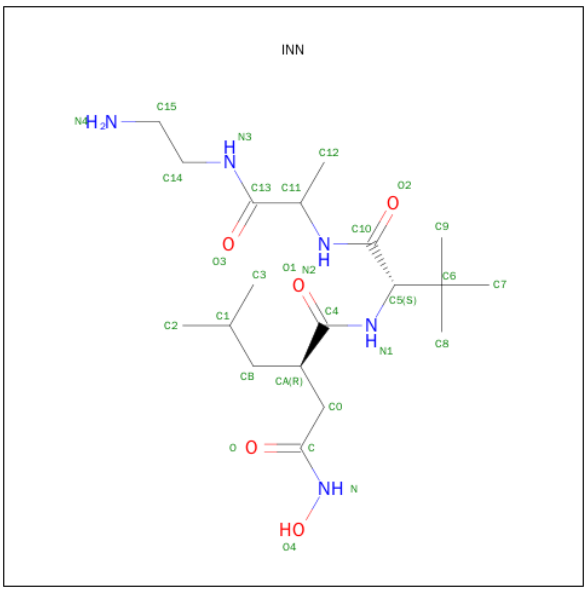
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	266	ALA	SER	ENGINEERED	UNP P78536
I	428	GLU	ASP	CONFLICT	UNP P78536
I	452	GLN	ASN	ENGINEERED	UNP P78536

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is N-{(2R)-2-[2-(HYDROXYAMINO)-2-OXOETHYL]-4-METHYLPENTANOYL}-3-METHYL-L-VALYL-N-(2-AMINOETHYL)-L-ALANINAMIDE (three-letter code: INN) (formula: $C_{19}H_{37}N_5O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 29 19 5 5	0	0
5	C	1	Total C N O 29 19 5 5	0	0
5	E	1	Total C N O 29 19 5 5	0	0
5	I	1	Total C N O 29 19 5 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	572	Total O 572 572	0	0
6	C	442	Total O 442 442	0	0
6	E	368	Total O 368 368	0	0
6	I	238	Total O 238 238	0	0

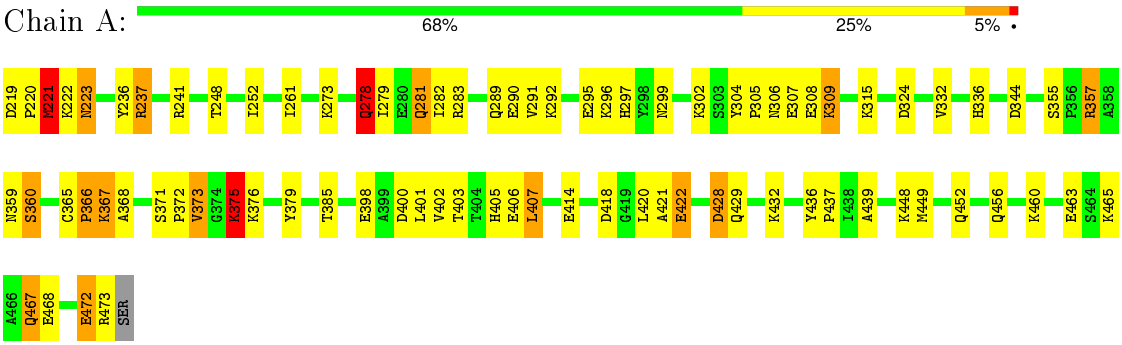
3 Residue-property plots (i)

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

Note EDS was not executed.

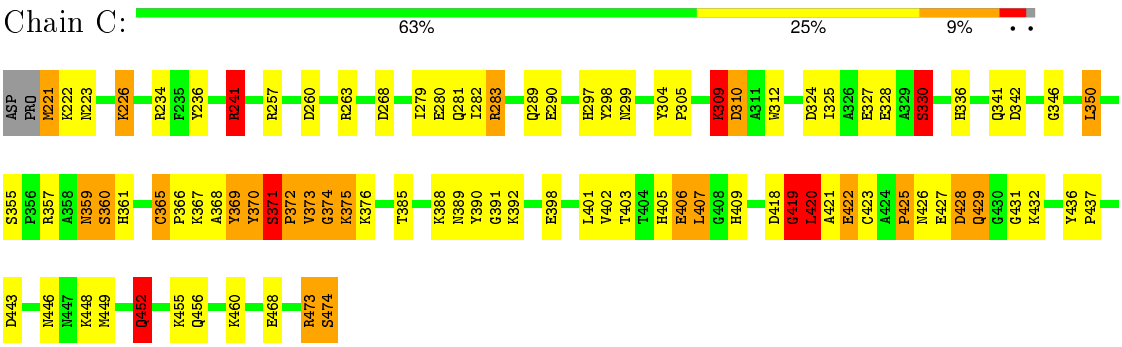
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain A:



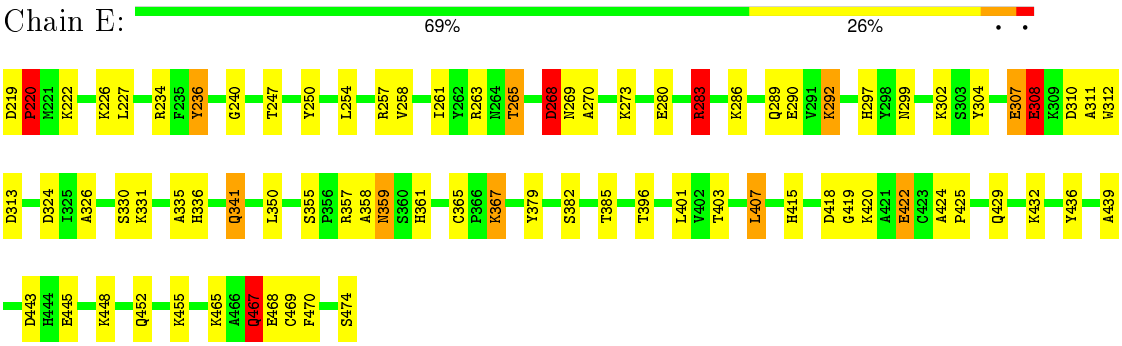
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain C:



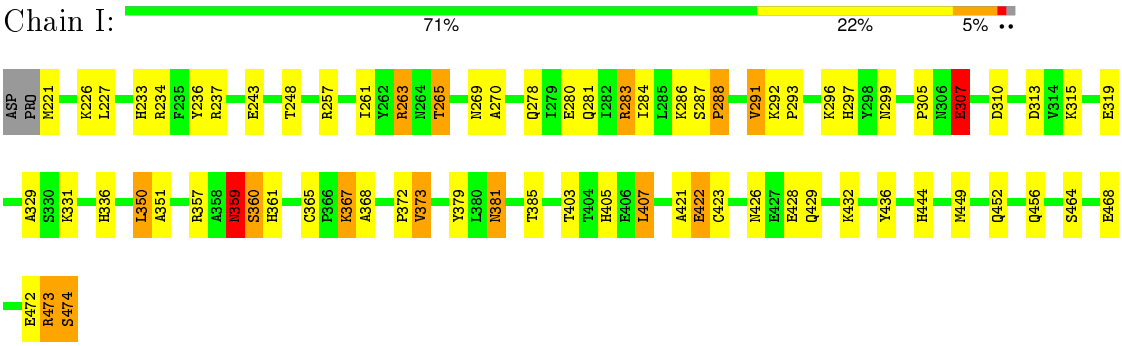
• Molecule 2: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain E:



• Molecule 3: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.38Å 126.27Å 81.27Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.00)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: ZN, INN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	1/2071 (0.0%)	1.43	16/2795 (0.6%)
1	C	1.29	13/2056 (0.6%)	2.03	52/2773 (1.9%)
2	E	0.81	2/2074 (0.1%)	1.60	33/2798 (1.2%)
3	I	0.80	4/2062 (0.2%)	1.54	25/2781 (0.9%)
All	All	0.93	20/8263 (0.2%)	1.67	126/11147 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	7
2	E	0	2
3	I	0	3
All	All	0	14

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	420	LEU	C-N	-29.95	0.65	1.34
1	C	376	LYS	C-N	-15.38	0.98	1.34
1	C	452	GLN	C-N	-14.60	1.00	1.34
1	C	374	GLY	N-CA	12.40	1.64	1.46
1	A	376	LYS	C-N	-10.51	1.09	1.34
1	C	371	SER	N-CA	-10.13	1.26	1.46
2	E	326	ALA	C-N	-7.94	1.15	1.34
3	I	368	ALA	C-N	-7.76	1.16	1.34
1	C	373	VAL	C-N	7.41	1.46	1.33
1	C	373	VAL	C-O	-7.24	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	307	GLU	C-N	-7.12	1.17	1.34
1	C	468	GLU	C-N	7.04	1.50	1.34
2	E	455	LYS	C-N	-7.00	1.18	1.34
3	I	292	LYS	C-N	6.75	1.47	1.34
1	C	426	ASN	C-N	-6.68	1.18	1.34
1	C	419	GLY	C-N	6.45	1.48	1.34
3	I	444	HIS	C-N	-6.02	1.20	1.34
1	C	422	GLU	C-N	-6.02	1.20	1.34
1	C	371	SER	C-O	5.79	1.34	1.23
1	C	372	PRO	CA-CB	-5.23	1.43	1.53

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	452	GLN	O-C-N	-28.28	77.45	122.70
1	C	419	GLY	O-C-N	-25.11	82.52	122.70
1	C	420	LEU	O-C-N	-22.23	87.13	122.70
1	C	369	TYR	O-C-N	21.44	157.01	122.70
1	C	420	LEU	C-N-CA	21.12	174.51	121.70
1	C	420	LEU	CA-C-N	15.02	150.24	117.20
1	C	369	TYR	CA-C-N	-14.42	85.47	117.20
1	C	241	ARG	CD-NE-CZ	14.17	143.44	123.60
1	C	452	GLN	CA-C-N	13.99	147.97	117.20
1	C	373	VAL	O-C-N	-13.29	100.61	123.20
1	C	283	ARG	NE-CZ-NH2	-13.20	113.70	120.30
2	E	467	GLN	C-N-CA	13.11	154.47	121.70
2	E	263	ARG	NE-CZ-NH1	11.95	126.28	120.30
3	I	473	ARG	NE-CZ-NH2	-11.88	114.36	120.30
3	I	257	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	C	376	LYS	O-C-N	-11.30	104.62	122.70
1	C	370	TYR	O-C-N	11.19	140.60	122.70
3	I	263	ARG	CD-NE-CZ	11.11	139.16	123.60
1	C	376	LYS	C-N-CA	10.77	148.63	121.70
2	E	263	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	C	428	ASP	N-CA-CB	10.09	128.77	110.60
1	C	310	ASP	CB-CG-OD1	-10.03	109.28	118.30
1	C	426	ASN	C-N-CA	10.01	146.72	121.70
1	C	373	VAL	CA-C-N	9.86	135.92	116.20
3	I	307	GLU	CA-C-N	9.82	138.80	117.20
3	I	257	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	418	ASP	CB-CG-OD2	9.29	126.67	118.30
3	I	368	ALA	O-C-N	9.28	137.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	LYS	O-C-N	-8.91	108.45	122.70
1	C	373	VAL	CB-CA-C	8.89	128.29	111.40
3	I	283	ARG	NE-CZ-NH2	-8.73	115.94	120.30
3	I	307	GLU	O-C-N	-8.63	108.90	122.70
1	C	234	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	E	283	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	E	283	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	473	ARG	NE-CZ-NH2	8.44	124.52	120.30
2	E	467	GLN	CA-C-O	8.38	137.70	120.10
1	C	426	ASN	O-C-N	-8.37	109.31	122.70
2	E	467	GLN	O-C-N	-8.04	109.83	122.70
3	I	263	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	268	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	324	ASP	CB-CG-OD2	7.93	125.44	118.30
1	C	370	TYR	CA-C-N	-7.91	99.79	117.20
2	E	311	ALA	N-CA-CB	-7.91	99.03	110.10
2	E	220	PRO	N-CA-C	7.64	131.97	112.10
3	I	234	ARG	NE-CZ-NH1	7.56	124.08	120.30
3	I	449	MET	CA-CB-CG	7.54	126.12	113.30
1	C	260	ASP	CB-CG-OD1	7.42	124.98	118.30
2	E	467	GLN	N-CA-CB	7.37	123.87	110.60
2	E	310	ASP	CB-CG-OD1	-7.36	111.68	118.30
3	I	473	ARG	CD-NE-CZ	7.24	133.73	123.60
2	E	313	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	C	390	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	A	344	ASP	CB-CG-OD1	7.02	124.62	118.30
2	E	304	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	C	376	LYS	CA-C-N	6.93	132.44	117.20
3	I	234	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	428	ASP	CB-CG-OD1	6.75	124.37	118.30
1	C	372	PRO	N-CA-CB	6.74	111.39	103.30
1	A	366	PRO	C-N-CA	6.68	138.39	121.70
3	I	237	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	369	TYR	C-N-CA	6.59	138.19	121.70
3	I	310	ASP	CB-CG-OD1	-6.58	112.38	118.30
3	I	473	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	E	268	ASP	CB-CA-C	-6.47	97.45	110.40
1	C	298	TYR	CB-CG-CD2	-6.31	117.22	121.00
2	E	455	LYS	CA-C-O	-6.28	106.92	120.10
1	C	368	ALA	O-C-N	-6.27	112.67	122.70
2	E	443	ASP	CB-CG-OD2	-6.26	112.66	118.30
2	E	326	ALA	CA-C-O	-6.24	106.99	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	359	ASN	N-CA-CB	-6.14	99.55	110.60
2	E	418	ASP	N-CA-CB	6.12	121.62	110.60
1	C	236	TYR	CB-CG-CD1	6.04	124.62	121.00
1	C	371	SER	CA-C-O	-5.98	107.54	120.10
3	I	359	ASN	N-CA-CB	5.94	121.30	110.60
1	C	290	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	C	310	ASP	OD1-CG-OD2	5.91	134.53	123.30
1	C	236	TYR	CB-CG-CD2	-5.89	117.47	121.00
2	E	419	GLY	N-CA-C	-5.87	98.42	113.10
3	I	305	PRO	CA-N-CD	-5.83	103.34	111.50
2	E	358	ALA	CA-C-O	5.76	132.20	120.10
2	E	250	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	I	243	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	A	304	TYR	CA-C-O	-5.61	108.32	120.10
1	A	400	ASP	CB-CG-OD2	-5.61	113.25	118.30
3	I	305	PRO	N-CD-CG	5.60	111.60	103.20
2	E	468	GLU	N-CA-C	-5.59	95.91	111.00
1	A	368	ALA	N-CA-C	5.57	126.05	111.00
1	C	330	SER	CB-CA-C	-5.57	99.51	110.10
2	E	324	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	C	283	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	414	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	C	324	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	C	257	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	443	ASP	CB-CG-OD1	5.45	123.20	118.30
3	I	405	HIS	CG-CD2-NE2	-5.43	98.88	109.20
1	A	278	GLN	CB-CA-C	-5.42	99.56	110.40
2	E	304	TYR	CB-CG-CD1	5.42	124.25	121.00
2	E	341	GLN	OE1-CD-NE2	5.41	134.35	121.90
1	A	357	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	305	PRO	N-CD-CG	5.34	111.22	103.20
1	C	406	GLU	OE1-CD-OE2	-5.32	116.92	123.30
2	E	257	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	E	227	LEU	CB-CA-C	-5.30	100.13	110.20
2	E	415	HIS	CG-CD2-NE2	-5.29	99.15	109.20
3	I	237	ARG	NE-CZ-NH2	-5.27	117.66	120.30
3	I	379	TYR	CB-CG-CD1	-5.22	117.87	121.00
3	I	313	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	310	ASP	CB-CA-C	5.19	120.78	110.40
2	E	236	TYR	CA-CB-CG	5.18	123.25	113.40
1	C	473	ARG	NE-CZ-NH1	-5.18	117.71	120.30
2	E	361	HIS	N-CA-CB	5.16	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	304	TYR	CA-C-O	-5.13	109.33	120.10
1	A	428	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	405	HIS	CG-CD2-NE2	-5.11	99.49	109.20
3	I	368	ALA	CA-C-O	-5.07	109.46	120.10
1	A	405	HIS	CG-CD2-NE2	-5.05	99.60	109.20
1	C	373	VAL	N-CA-C	-5.05	97.35	111.00
2	E	307	GLU	CA-C-N	5.05	128.32	117.20
1	C	409	HIS	CG-CD2-NE2	-5.04	99.63	109.20
1	C	350	LEU	CB-CG-CD2	5.03	119.55	111.00
1	C	305	PRO	N-CD-CG	5.03	110.75	103.20
1	C	260	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	305	PRO	CA-N-CD	-5.02	104.47	111.50
1	C	309	LYS	CB-CA-C	5.00	120.41	110.40
2	E	468	GLU	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	Mainchain
1	A	375	LYS	Mainchain
1	C	371	SER	Mainchain,Peptide
1	C	375	LYS	Peptide
1	C	419	GLY	Mainchain
1	C	420	LEU	Peptide
1	C	425	PRO	Mainchain
1	C	452	GLN	Mainchain
2	E	268	ASP	Mainchain
2	E	467	GLN	Peptide
3	I	270	ALA	Mainchain
3	I	291	VAL	Mainchain
3	I	307	GLU	Mainchain

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	A	2025	0	1937	67	2
1	C	2012	0	1915	58	4
2	E	2028	0	1937	55	2
3	I	2017	0	1931	50	4
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	29	0	34	1	1
5	C	29	0	35	1	0
5	E	29	0	35	1	1
5	I	29	0	35	0	1
6	A	572	0	0	21	18
6	C	442	0	0	16	8
6	E	368	0	0	9	18
6	I	238	0	0	8	9
All	All	9822	0	7859	231	34

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 15.

All (231) 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)
3:I:350:LEU:HG	6:I:1289:HOH:O	1.60	1.00
3:I:281:GLN:HE21	3:I:283:ARG:HE	0.99	0.97
1:C:279:ILE:HG23	6:C:838:HOH:O	1.64	0.95
1:A:219:ASP:N	1:A:467:GLN:HE22	1.67	0.91
1:C:281:GLN:HE21	1:C:283:ARG:NE	1.68	0.91
3:I:278:GLN:HE22	3:I:474:SER:H	0.95	0.89
1:A:449:MET:HG3	6:A:676:HOH:O	1.75	0.87
1:C:388:LYS:HG2	6:C:879:HOH:O	1.75	0.86
3:I:281:GLN:NE2	3:I:283:ARG:HH21	1.74	0.84
1:A:278:GLN:HE22	1:A:473:ARG:NH1	1.76	0.84
1:C:223:ASN:ND2	1:C:473:ARG:HH12	1.75	0.83
1:C:223:ASN:HD21	1:C:473:ARG:HH12	1.25	0.83
1:A:219:ASP:HB3	1:A:222:LYS:H	1.43	0.82
1:C:346:GLY:HA2	1:C:389:ASN:HD21	1.45	0.82
2:E:467:GLN:HB2	2:E:470:PHE:O	1.79	0.81
1:C:281:GLN:NE2	1:C:283:ARG:NE	2.29	0.80
1:A:279:ILE:HD13	1:A:282:ILE:HD11	1.62	0.80
3:I:278:GLN:HE22	3:I:474:SER:N	1.78	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:302:LYS:HB3	2:E:307:GLU:HG3	1.64	0.78
1:C:297:HIS:HD2	1:C:299:ASN:H	1.30	0.78
3:I:297:HIS:HD2	3:I:299:ASN:H	1.33	0.76
3:I:281:GLN:NE2	3:I:283:ARG:HE	1.80	0.76
2:E:307:GLU:O	2:E:308:GLU:HB3	1.83	0.76
3:I:281:GLN:HE22	3:I:283:ARG:HH21	1.34	0.74
3:I:297:HIS:CD2	3:I:299:ASN:H	2.06	0.74
3:I:281:GLN:HE21	3:I:283:ARG:NE	1.81	0.74
3:I:278:GLN:NE2	3:I:474:SER:H	1.80	0.74
1:A:297:HIS:HD2	1:A:299:ASN:H	1.35	0.74
1:C:473:ARG:O	1:C:474:SER:HB2	1.89	0.73
1:A:279:ILE:HG21	1:A:282:ILE:HG13	1.70	0.72
3:I:381:ASN:HD22	3:I:381:ASN:H	1.38	0.71
2:E:359:ASN:HB3	2:E:367:LYS:CD	2.21	0.70
2:E:297:HIS:CD2	2:E:299:ASN:H	2.09	0.70
2:E:297:HIS:HD2	2:E:299:ASN:H	1.37	0.70
1:A:315:LYS:HB3	6:A:991:HOH:O	1.90	0.69
3:I:372:PRO:O	3:I:373:VAL:HB	1.93	0.69
2:E:467:GLN:HA	2:E:470:PHE:H	1.56	0.69
1:C:425:PRO:HB3	1:C:429:GLN:HB3	1.74	0.69
3:I:473:ARG:O	3:I:474:SER:HB2	1.93	0.68
2:E:269:ASN:HD21	2:E:452:GLN:HE22	1.39	0.68
1:C:281:GLN:NE2	1:C:283:ARG:HE	1.91	0.68
1:A:297:HIS:CD2	1:A:299:ASN:H	2.11	0.68
1:A:278:GLN:HE22	1:A:473:ARG:HH11	1.41	0.66
1:A:220:PRO:HD3	6:A:1046:HOH:O	1.95	0.66
1:C:342:ASP:OD1	6:C:614:HOH:O	2.14	0.66
3:I:227:LEU:HB3	6:I:2206:HOH:O	1.96	0.66
1:A:282:ILE:HB	6:A:944:HOH:O	1.95	0.66
3:I:269:ASN:HD21	3:I:452:GLN:HE22	1.44	0.65
1:C:312:TRP:H	1:C:341:GLN:NE2	1.94	0.64
1:C:297:HIS:CD2	1:C:299:ASN:H	2.14	0.64
3:I:359:ASN:HA	3:I:367:LYS:HD3	1.80	0.64
3:I:360:SER:H	3:I:367:LYS:HD3	1.63	0.64
1:A:403:THR:HG22	1:A:407:LEU:HD22	1.80	0.63
5:C:2:INN:H142	6:C:798:HOH:O	2.00	0.62
2:E:261:ILE:O	2:E:265:THR:HG22	2.00	0.62
2:E:234:ARG:NH1	6:E:805:HOH:O	2.33	0.61
1:A:278:GLN:NE2	1:A:473:ARG:NH1	2.48	0.61
2:E:312:TRP:H	2:E:341:GLN:NE2	1.99	0.61
2:E:307:GLU:O	2:E:308:GLU:OE1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLN:HG3	6:A:923:HOH:O	2.02	0.60
1:C:281:GLN:HG3	6:C:738:HOH:O	2.00	0.60
3:I:281:GLN:NE2	3:I:283:ARG:NH2	2.50	0.59
1:C:421:ALA:HB1	1:C:423:CYS:N	2.17	0.59
3:I:248:THR:OG1	3:I:284:ILE:HD11	2.02	0.59
2:E:307:GLU:O	2:E:308:GLU:CB	2.51	0.59
1:A:357:ARG:O	1:A:360:SER:HB3	2.02	0.59
1:A:220:PRO:HG2	6:A:815:HOH:O	2.03	0.59
1:C:223:ASN:HD21	1:C:473:ARG:NH1	1.97	0.58
3:I:359:ASN:HA	3:I:367:LYS:CE	2.34	0.58
2:E:467:GLN:HA	2:E:469:CYS:N	2.19	0.58
1:C:226:LYS:HB3	1:C:280:GLU:HB2	1.85	0.58
3:I:233:HIS:H	3:I:299:ASN:HD21	1.52	0.57
3:I:429:GLN:NE2	6:I:1353:HOH:O	2.38	0.57
2:E:222:LYS:CE	2:E:467:GLN:HB3	2.35	0.56
2:E:226:LYS:HB3	2:E:280:GLU:HB2	1.86	0.56
1:C:388:LYS:HE2	6:C:879:HOH:O	2.05	0.56
2:E:222:LYS:CD	2:E:467:GLN:HB3	2.36	0.56
1:A:241:ARG:HB3	1:A:241:ARG:HH11	1.69	0.56
1:C:401:LEU:HD21	1:C:448:LYS:HG2	1.87	0.56
1:C:336:HIS:HE1	1:C:385:THR:OG1	1.87	0.56
3:I:329:ALA:HB1	3:I:381:ASN:HD21	1.70	0.55
1:A:219:ASP:N	1:A:467:GLN:NE2	2.47	0.55
2:E:336:HIS:HE1	2:E:385:THR:OG1	1.90	0.55
2:E:240:GLY:HA3	2:E:247:THR:OG1	2.08	0.54
1:A:372:PRO:O	1:A:373:VAL:HB	2.07	0.54
3:I:226:LYS:HB3	3:I:280:GLU:HB2	1.89	0.54
1:A:302:LYS:HG2	6:A:539:HOH:O	2.07	0.54
2:E:269:ASN:HD21	2:E:452:GLN:NE2	2.06	0.53
2:E:258:VAL:HG13	6:E:827:HOH:O	2.08	0.53
2:E:403:THR:HG22	2:E:407:LEU:HD22	1.89	0.53
1:C:456:GLN:O	1:C:460:LYS:HG3	2.09	0.53
2:E:467:GLN:HA	2:E:470:PHE:N	2.22	0.53
3:I:233:HIS:H	3:I:299:ASN:ND2	2.06	0.53
1:C:456:GLN:HG3	6:C:903:HOH:O	2.09	0.53
3:I:221:MET:HB3	3:I:472:GLU:HG2	1.91	0.53
1:A:336:HIS:HD2	6:A:569:HOH:O	1.90	0.53
3:I:261:ILE:O	3:I:265:THR:HG22	2.08	0.52
1:A:308:GLU:HG2	1:A:309:LYS:HE2	1.90	0.52
2:E:467:GLN:H	2:E:470:PHE:HB2	1.75	0.52
3:I:357:ARG:O	3:I:360:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:381:ASN:N	3:I:381:ASN:HD22	2.06	0.52
1:C:403:THR:HG22	1:C:407:LEU:HD22	1.91	0.52
2:E:359:ASN:HB3	2:E:367:LYS:HD2	1.92	0.52
2:E:331:LYS:HE2	6:E:821:HOH:O	2.10	0.51
1:A:336:HIS:HE1	1:A:385:THR:OG1	1.92	0.51
2:E:222:LYS:HE2	2:E:467:GLN:HB3	1.92	0.51
1:A:223:ASN:H	1:A:223:ASN:HD22	1.57	0.51
1:A:359:ASN:HB3	6:A:896:HOH:O	2.10	0.50
1:A:468:GLU:HG2	6:A:790:HOH:O	2.11	0.50
1:A:222:LYS:HE2	6:A:814:HOH:O	2.12	0.50
2:E:467:GLN:NE2	2:E:470:PHE:O	2.44	0.50
3:I:421:ALA:O	3:I:423:CYS:N	2.39	0.50
2:E:336:HIS:HD2	6:E:485:HOH:O	1.94	0.49
1:A:237:ARG:HH11	1:A:237:ARG:HA	1.77	0.49
2:E:268:ASP:HB3	2:E:270:ALA:H	1.77	0.49
1:C:391:GLY:N	6:C:879:HOH:O	2.37	0.49
3:I:432:LYS:HD3	3:I:436:TYR:CD2	2.47	0.49
1:A:306:ASN:HB3	1:A:308:GLU:OE2	2.12	0.49
1:C:419:GLY:O	1:C:421:ALA:N	2.45	0.49
1:C:402:VAL:O	1:C:406:GLU:HG2	2.12	0.49
1:A:292:LYS:HB2	1:A:295:GLU:CD	2.32	0.49
1:C:281:GLN:NE2	1:C:283:ARG:CZ	2.76	0.49
3:I:359:ASN:HA	3:I:367:LYS:CD	2.41	0.48
2:E:429:GLN:HG3	6:E:770:HOH:O	2.12	0.48
1:A:452:GLN:HE21	1:A:456:GLN:HG3	1.77	0.48
3:I:287:SER:HB2	3:I:288:PRO:HD2	1.95	0.48
1:A:359:ASN:HB2	6:A:895:HOH:O	2.14	0.48
1:A:398:GLU:HA	1:A:401:LEU:HD12	1.95	0.48
1:A:241:ARG:HB3	1:A:241:ARG:NH1	2.29	0.47
2:E:432:LYS:HD2	2:E:436:TYR:CD1	2.50	0.47
1:C:221:MET:HG2	1:C:222:LYS:N	2.29	0.47
2:E:307:GLU:HB3	6:E:627:HOH:O	2.14	0.47
2:E:270:ALA:O	2:E:273:LYS:HE2	2.15	0.47
3:I:315:LYS:HA	6:I:1289:HOH:O	2.14	0.47
1:A:436:TYR:CG	1:A:437:PRO:HD2	2.50	0.47
1:A:460:LYS:HD3	1:A:460:LYS:HA	1.73	0.47
3:I:315:LYS:O	3:I:319:GLU:HG3	2.15	0.46
1:A:448:LYS:HB2	6:A:933:HOH:O	2.13	0.46
1:A:332:VAL:O	1:A:366:PRO:HG3	2.16	0.46
2:E:467:GLN:HA	2:E:469:CYS:H	1.80	0.46
1:A:241:ARG:HG3	6:A:983:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:GLN:HG2	1:C:297:HIS:CG	2.51	0.46
1:C:428:ASP:O	1:C:429:GLN:HB2	2.16	0.46
2:E:439:ALA:HA	5:E:2:INN:H21	1.98	0.46
3:I:336:HIS:HE1	3:I:385:THR:OG1	1.99	0.46
2:E:359:ASN:HB3	2:E:367:LYS:HD3	1.98	0.46
2:E:424:ALA:N	2:E:425:PRO:HD3	2.30	0.45
2:E:292:LYS:HD3	2:E:292:LYS:HA	1.87	0.45
1:C:241:ARG:HA	1:C:241:ARG:HD2	1.84	0.45
1:A:371:SER:OG	1:A:373:VAL:O	2.34	0.45
3:I:336:HIS:HD2	6:I:1169:HOH:O	1.99	0.45
3:I:359:ASN:HA	3:I:367:LYS:HE2	1.97	0.45
1:A:299:ASN:ND2	6:A:865:HOH:O	2.50	0.45
3:I:236:TYR:CZ	3:I:286:LYS:HG2	2.52	0.45
1:A:367:LYS:HD3	6:A:970:HOH:O	2.16	0.44
1:A:297:HIS:HE1	6:A:747:HOH:O	2.00	0.44
1:C:456:GLN:HG3	6:C:683:HOH:O	2.17	0.44
1:A:375:LYS:HG3	6:A:961:HOH:O	2.17	0.44
2:E:330:SER:HB3	2:E:379:TYR:CE2	2.53	0.44
2:E:222:LYS:HE2	2:E:467:GLN:HG2	2.00	0.44
3:I:359:ASN:CA	3:I:367:LYS:HD3	2.45	0.44
1:C:398:GLU:O	1:C:402:VAL:HG23	2.17	0.44
1:C:327:GLU:O	1:C:330:SER:HB2	2.17	0.44
1:A:366:PRO:HB2	1:A:379:TYR:CD2	2.53	0.44
2:E:283:ARG:HG2	6:E:582:HOH:O	2.18	0.44
1:C:421:ALA:HB1	1:C:423:CYS:HB2	1.98	0.44
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.31	0.44
1:C:325:ILE:HD11	1:C:328:GLU:OE1	2.17	0.44
1:C:428:ASP:O	1:C:429:GLN:CB	2.65	0.43
1:C:309:LYS:HG3	6:C:754:HOH:O	2.18	0.43
1:C:223:ASN:HD21	1:C:473:ARG:HH22	1.65	0.43
1:A:223:ASN:H	1:A:223:ASN:ND2	2.14	0.43
1:A:281:GLN:HG3	1:A:282:ILE:N	2.34	0.43
2:E:289:GLN:HG2	2:E:297:HIS:CG	2.53	0.43
1:C:336:HIS:HD2	6:C:609:HOH:O	2.02	0.43
1:A:421:ALA:HA	6:A:1022:HOH:O	2.17	0.43
3:I:422:GLU:H	3:I:422:GLU:HG3	1.59	0.43
1:C:421:ALA:CB	1:C:423:CYS:HB2	2.49	0.43
1:A:402:VAL:O	1:A:406:GLU:HG2	2.18	0.43
1:C:446:ASN:HA	1:C:449:MET:CE	2.49	0.43
1:C:389:ASN:ND2	6:C:614:HOH:O	2.44	0.43
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:LYS:HD2	6:C:619:HOH:O	2.17	0.43
1:C:431:GLY:HA2	6:C:795:HOH:O	2.19	0.42
1:A:221:MET:O	1:A:472:GLU:HA	2.19	0.42
1:A:261:ILE:HD11	1:A:448:LYS:HD3	2.00	0.42
2:E:236:TYR:CZ	2:E:286:LYS:HG2	2.54	0.42
2:E:401:LEU:HD21	2:E:448:LYS:HG2	2.02	0.42
2:E:307:GLU:N	6:E:625:HOH:O	2.44	0.42
2:E:297:HIS:HE1	6:E:608:HOH:O	2.02	0.42
3:I:360:SER:N	3:I:367:LYS:HD3	2.33	0.42
1:C:357:ARG:O	1:C:360:SER:HB3	2.20	0.42
1:A:355:SER:HB3	1:A:360:SER:HB2	2.01	0.42
1:A:452:GLN:NE2	1:A:456:GLN:HG3	2.34	0.42
1:A:421:ALA:O	1:A:422:GLU:CB	2.66	0.42
1:A:439:ALA:HA	5:A:2:INN:H21	2.01	0.42
1:C:361:HIS:CE1	1:C:367:LYS:HD3	2.55	0.42
1:C:279:ILE:HG21	1:C:282:ILE:HG13	2.02	0.42
1:A:289:GLN:HG2	1:A:297:HIS:CG	2.54	0.42
3:I:421:ALA:O	6:I:1350:HOH:O	2.20	0.42
1:C:418:ASP:OD2	1:C:436:TYR:OH	2.38	0.42
1:A:372:PRO:O	1:A:373:VAL:CB	2.67	0.42
1:C:446:ASN:HA	1:C:449:MET:HE3	2.02	0.42
2:E:335:ALA:O	2:E:382:SER:HA	2.20	0.41
1:C:403:THR:O	1:C:407:LEU:HB2	2.20	0.41
1:A:456:GLN:NE2	6:A:805:HOH:O	2.53	0.41
3:I:286:LYS:NZ	6:I:2208:HOH:O	2.47	0.41
2:E:254:LEU:C	2:E:254:LEU:HD23	2.40	0.41
2:E:422:GLU:HG3	2:E:422:GLU:H	1.15	0.41
2:E:219:ASP:HA	2:E:220:PRO:HD3	1.84	0.41
3:I:456:GLN:HG3	6:I:2223:HOH:O	2.19	0.41
1:C:297:HIS:HE1	6:C:533:HOH:O	2.02	0.41
1:A:220:PRO:O	1:A:221:MET:HB2	2.21	0.41
1:A:432:LYS:HD3	1:A:436:TYR:CD2	2.55	0.41
3:I:403:THR:HG22	3:I:407:LEU:HD22	2.02	0.41
1:A:302:LYS:HB3	1:A:307:GLU:HG2	2.01	0.41
1:C:436:TYR:CD1	1:C:437:PRO:HD2	2.55	0.41
2:E:234:ARG:HH11	2:E:234:ARG:HD3	1.72	0.41
1:A:236:TYR:HD2	1:A:237:ARG:HD2	1.85	0.41
1:C:359:ASN:HA	1:C:359:ASN:HD22	1.65	0.41
2:E:467:GLN:N	2:E:470:PHE:H	2.19	0.41
2:E:222:LYS:CG	2:E:467:GLN:HB3	2.51	0.41
3:I:350:LEU:CD1	3:I:351:ALA:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:NH1	6:A:700:HOH:O	2.54	0.41
1:C:361:HIS:ND1	1:C:367:LYS:HD3	2.36	0.41
1:A:248:THR:O	1:A:252:ILE:HG13	2.21	0.40
3:I:297:HIS:HD2	3:I:299:ASN:N	2.08	0.40
3:I:381:ASN:ND2	3:I:381:ASN:H	2.11	0.40
1:C:365:CYS:HA	1:C:366:PRO:HD2	1.89	0.40
1:C:342:ASP:CG	6:C:879:HOH:O	2.59	0.40
2:E:357:ARG:O	2:E:359:ASN:N	2.55	0.40

All (34) 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)
1:C:452:GLN:CD	6:A:1012:HOH:O[1_655]	1.08	1.12
1:C:452:GLN:CG	6:A:1012:HOH:O[1_655]	1.20	1.00
6:A:920:HOH:O	6:E:606:HOH:O[2_546]	1.55	0.65
6:A:710:HOH:O	6:I:1189:HOH:O[2_656]	1.56	0.64
6:A:600:HOH:O	6:E:628:HOH:O[2_546]	1.66	0.54
3:I:426:ASN:CB	6:A:1011:HOH:O[2_545]	1.69	0.51
5:I:2:INN:N4	6:C:862:HOH:O[2_545]	1.85	0.35
6:A:733:HOH:O	6:E:737:HOH:O[2_646]	1.86	0.34
1:C:452:GLN:NE2	6:A:1012:HOH:O[1_655]	1.89	0.31
6:A:870:HOH:O	6:I:1257:HOH:O[2_656]	1.89	0.31
1:C:452:GLN:OE1	6:A:1012:HOH:O[1_655]	1.91	0.29
6:A:876:HOH:O	6:E:730:HOH:O[2_646]	1.94	0.26
6:E:822:HOH:O	6:I:1234:HOH:O[2_555]	1.95	0.25
6:C:823:HOH:O	6:I:1194:HOH:O[2_655]	1.98	0.22
6:A:721:HOH:O	6:E:521:HOH:O[2_646]	1.98	0.22
3:I:331:LYS:CD	6:E:751:HOH:O[2_646]	2.00	0.20
3:I:421:ALA:CB	6:C:593:HOH:O[2_545]	2.02	0.18
6:E:822:HOH:O	6:I:1229:HOH:O[2_555]	2.03	0.17
1:A:421:ALA:CB	6:E:638:HOH:O[2_546]	2.03	0.17
6:A:983:HOH:O	6:E:521:HOH:O[2_646]	2.04	0.16
6:A:947:HOH:O	6:E:729:HOH:O[2_646]	2.05	0.15
2:E:429:GLN:NE2	6:I:1244:HOH:O[2_656]	2.07	0.13
3:I:456:GLN:OE1	6:E:715:HOH:O[2_545]	2.09	0.11
5:E:2:INN:N4	6:C:907:HOH:O[2_656]	2.10	0.10
6:A:530:HOH:O	6:I:1252:HOH:O[2_656]	2.10	0.10
6:C:857:HOH:O	6:I:1287:HOH:O[2_555]	2.14	0.06
6:A:920:HOH:O	6:E:605:HOH:O[2_546]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:917:HOH:O	6:E:620:HOH:O[2_546]	2.16	0.04
6:C:847:HOH:O	6:E:589:HOH:O[2_545]	2.17	0.03
1:A:421:ALA:N	6:E:638:HOH:O[2_546]	2.17	0.03
5:A:2:INN:N4	6:E:602:HOH:O[2_546]	2.17	0.03
2:E:290:GLU:CD	6:C:848:HOH:O[2_555]	2.18	0.02
6:A:505:HOH:O	6:E:737:HOH:O[2_646]	2.18	0.02
6:C:543:HOH:O	6:I:1279:HOH:O[2_555]	2.18	0.02

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	A	253/256 (99%)	241 (95%)	8 (3%)	4 (2%)	12 5
1	C	250/256 (98%)	228 (91%)	14 (6%)	8 (3%)	5 1
2	E	254/256 (99%)	238 (94%)	11 (4%)	5 (2%)	9 3
3	I	252/256 (98%)	243 (96%)	3 (1%)	6 (2%)	7 2
All	All	1009/1024 (98%)	950 (94%)	36 (4%)	23 (2%)	8 3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	373	VAL
1	C	370	TYR
1	C	371	SER
1	C	372	PRO
1	C	373	VAL
1	C	429	GLN
2	E	220	PRO
2	E	420	LYS
2	E	467	GLN

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Mol	Chain	Res	Type
3	I	359	ASN
3	I	422	GLU
3	I	428	GLU
1	A	420	LEU
1	C	369	TYR
2	E	308	GLU
1	A	365	CYS
1	C	365	CYS
2	E	365	CYS
3	I	365	CYS
3	I	293	PRO
3	I	373	VAL
1	C	374	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	218/219 (100%)	198 (91%)	20 (9%)	11 6
1	C	216/219 (99%)	195 (90%)	21 (10%)	10 5
2	E	218/219 (100%)	202 (93%)	16 (7%)	17 11
3	I	217/219 (99%)	202 (93%)	15 (7%)	19 13
All	All	869/876 (99%)	797 (92%)	72 (8%)	14 8

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	223	ASN
1	A	237	ARG
1	A	273	LYS
1	A	278	GLN
1	A	281	GLN
1	A	283	ARG
1	A	290	GLU

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Mol	Chain	Res	Type
1	A	291	VAL
1	A	296	LYS
1	A	309	LYS
1	A	360	SER
1	A	367	LYS
1	A	407	LEU
1	A	422	GLU
1	A	428	ASP
1	A	463	GLU
1	A	465	LYS
1	A	467	GLN
1	A	472	GLU
1	C	221	MET
1	C	226	LYS
1	C	241	ARG
1	C	263	ARG
1	C	309	LYS
1	C	310	ASP
1	C	330	SER
1	C	350	LEU
1	C	355	SER
1	C	359	ASN
1	C	360	SER
1	C	371	SER
1	C	375	LYS
1	C	407	LEU
1	C	420	LEU
1	C	422	GLU
1	C	427	GLU
1	C	432	LYS
1	C	452	GLN
1	C	455	LYS
1	C	474	SER
2	E	220	PRO
2	E	265	THR
2	E	268	ASP
2	E	283	ARG
2	E	292	LYS
2	E	308	GLU
2	E	350	LEU
2	E	355	SER
2	E	367	LYS

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Mol	Chain	Res	Type
2	E	396	THR
2	E	407	LEU
2	E	422	GLU
2	E	445	GLU
2	E	465	LYS
2	E	467	GLN
2	E	474	SER
3	I	263	ARG
3	I	265	THR
3	I	288	PRO
3	I	291	VAL
3	I	296	LYS
3	I	307	GLU
3	I	350	LEU
3	I	360	SER
3	I	361	HIS
3	I	367	LYS
3	I	381	ASN
3	I	407	LEU
3	I	464	SER
3	I	468	GLU
3	I	474	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	269	ASN
1	A	278	GLN
1	A	297	HIS
1	A	306	ASN
1	A	336	HIS
1	A	452	GLN
1	A	456	GLN
1	C	223	ASN
1	C	249	ASN
1	C	281	GLN
1	C	297	HIS
1	C	306	ASN
1	C	336	HIS
1	C	341	GLN
1	C	359	ASN

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Mol	Chain	Res	Type
1	C	389	ASN
1	C	429	GLN
1	C	456	GLN
2	E	264	ASN
2	E	297	HIS
2	E	336	HIS
2	E	341	GLN
2	E	452	GLN
3	I	278	GLN
3	I	281	GLN
3	I	297	HIS
3	I	299	ASN
3	I	336	HIS
3	I	381	ASN
3	I	429	GLN
3	I	452	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\|>2$
5	INN	A	2	4	28,28,28	3.31	5 (17%)	33,38,38	5.24	19 (57%)
5	INN	C	2	4	28,28,28	3.51	5 (17%)	33,38,38	5.16	19 (57%)
5	INN	E	2	4	28,28,28	3.42	5 (17%)	33,38,38	3.81	12 (36%)
5	INN	I	2	4	28,28,28	3.62	6 (21%)	33,38,38	4.65	18 (54%)

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
5	INN	A	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	C	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	E	2	4	1/1/9/13	0/40/40/40	0/0/0/0
5	INN	I	2	4	1/1/9/13	0/40/40/40	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	INN	C11-C13	-8.88	1.29	1.52
5	C	2	INN	C11-C13	-8.63	1.29	1.52
5	E	2	INN	C11-C13	-8.43	1.30	1.52
5	C	2	INN	C10-N2	-8.33	1.14	1.34
5	I	2	INN	C11-C13	-8.32	1.30	1.52
5	E	2	INN	C10-N2	-8.08	1.15	1.34
5	I	2	INN	C10-N2	-7.53	1.16	1.34
5	A	2	INN	C10-N2	-7.45	1.16	1.34
5	I	2	INN	C0-CA	-5.45	1.42	1.53
5	C	2	INN	C0-CA	-4.58	1.44	1.53
5	E	2	INN	C0-CA	-4.45	1.44	1.53
5	A	2	INN	C0-CA	-3.86	1.45	1.53
5	E	2	INN	O4-N	-2.81	1.34	1.39
5	A	2	INN	O4-N	-2.37	1.35	1.39
5	C	2	INN	C6-C5	2.04	1.59	1.55
5	I	2	INN	CA-C4	2.12	1.55	1.51
5	I	2	INN	C-N	2.14	1.34	1.32
5	A	2	INN	C4-N1	11.39	1.60	1.34
5	E	2	INN	C4-N1	11.74	1.61	1.34
5	C	2	INN	C4-N1	12.30	1.62	1.34
5	I	2	INN	C4-N1	13.06	1.64	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	INN	O3-C13-C11	-12.01	91.70	120.45
5	E	2	INN	O3-C13-C11	-11.87	92.04	120.45
5	A	2	INN	O3-C13-C11	-11.46	93.04	120.45
5	I	2	INN	O3-C13-C11	-11.10	93.88	120.45
5	A	2	INN	C5-N1-C4	-8.61	104.55	121.93
5	E	2	INN	CA-C0-C	-6.99	98.39	112.27
5	E	2	INN	C5-N1-C4	-6.76	108.28	121.93
5	A	2	INN	CA-C0-C	-6.53	99.30	112.27
5	C	2	INN	CA-C0-C	-6.52	99.32	112.27
5	I	2	INN	C5-N1-C4	-6.51	108.79	121.93
5	C	2	INN	O3-C13-N3	-6.47	110.09	123.08
5	A	2	INN	C14-N3-C13	-5.94	110.78	122.53
5	I	2	INN	O-C-C0	-5.90	112.68	121.30
5	A	2	INN	O3-C13-N3	-5.48	112.09	123.08
5	I	2	INN	CA-C0-C	-5.18	101.99	112.27
5	I	2	INN	O-C-N	-4.63	118.06	123.53
5	I	2	INN	O2-C10-C5	-4.53	114.43	121.16
5	C	2	INN	C5-N1-C4	-4.53	112.80	121.93
5	I	2	INN	C10-C5-N1	-4.49	99.35	108.94
5	I	2	INN	O3-C13-N3	-4.17	114.72	123.08
5	A	2	INN	O2-C10-C5	-4.06	115.14	121.16
5	A	2	INN	C10-C5-N1	-4.05	100.28	108.94
5	A	2	INN	O-C-C0	-3.91	115.60	121.30
5	C	2	INN	O-C-C0	-3.90	115.61	121.30
5	A	2	INN	O1-C4-N1	-3.73	115.63	122.93
5	E	2	INN	C6-C5-N1	-3.67	108.27	112.34
5	I	2	INN	C6-C5-C10	-3.39	109.40	112.83
5	E	2	INN	C6-C5-C10	-3.35	109.44	112.83
5	A	2	INN	C6-C5-N1	-3.18	108.82	112.34
5	C	2	INN	C6-C5-N1	-3.06	108.95	112.34
5	C	2	INN	O1-C4-CA	-2.98	118.25	122.12
5	C	2	INN	O2-C10-C5	-2.79	117.01	121.16
5	A	2	INN	C6-C5-C10	-2.77	110.02	112.83
5	C	2	INN	C6-C5-C10	-2.62	110.18	112.83
5	C	2	INN	O1-C4-N1	-2.62	117.81	122.93
5	A	2	INN	O1-C4-CA	-2.52	118.85	122.12
5	E	2	INN	O-C-N	-2.39	120.71	123.53
5	I	2	INN	O1-C4-N1	-2.29	118.44	122.93
5	I	2	INN	O1-C4-CA	-2.17	119.30	122.12
5	C	2	INN	C10-C5-N1	-2.17	104.30	108.94
5	E	2	INN	C10-C5-N1	-2.15	104.34	108.94
5	I	2	INN	C14-N3-C13	-2.05	118.48	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	INN	CA-C4-N1	2.00	119.47	116.30
5	I	2	INN	O2-C10-N2	2.02	126.88	122.93
5	C	2	INN	C14-N3-C13	2.06	126.60	122.53
5	I	2	INN	C5-C10-N2	2.15	118.49	115.46
5	C	2	INN	C12-C11-C13	2.16	114.47	110.19
5	A	2	INN	C12-C11-N2	2.28	114.62	110.31
5	E	2	INN	C12-C11-N2	2.89	115.77	110.31
5	C	2	INN	C11-N2-C10	3.14	128.46	121.27
5	E	2	INN	C12-C11-C13	3.16	116.44	110.19
5	C	2	INN	CA-C4-N1	3.56	121.93	116.30
5	A	2	INN	C11-N2-C10	3.80	129.99	121.27
5	C	2	INN	C5-C10-N2	4.07	121.20	115.46
5	A	2	INN	C5-C10-N2	4.10	121.24	115.46
5	I	2	INN	O4-N-C	5.14	127.33	119.56
5	A	2	INN	CA-C4-N1	5.41	124.85	116.30
5	E	2	INN	C13-C11-N2	6.30	127.41	111.67
5	A	2	INN	C13-C11-N2	6.90	128.89	111.67
5	C	2	INN	C13-C11-N2	7.41	130.17	111.67
5	E	2	INN	O4-N-C	7.84	131.41	119.56
5	E	2	INN	C11-C13-N3	8.32	134.61	116.43
5	I	2	INN	C13-C11-N2	8.40	132.64	111.67
5	C	2	INN	O4-N-C	9.58	134.06	119.56
5	A	2	INN	O4-N-C	10.31	135.16	119.56
5	I	2	INN	C11-C13-N3	15.95	151.27	116.43
5	A	2	INN	C11-C13-N3	16.67	152.85	116.43
5	C	2	INN	C11-C13-N3	18.98	157.88	116.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2	INN	C11
5	E	2	INN	C11
5	C	2	INN	C11
5	I	2	INN	C11

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	INN	1	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	INN	1	0
5	E	2	INN	1	1
5	I	2	INN	0	1

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 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.