Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:51 PM GMT

PDB ID	:	1CTP
Title	:	STRUCTURE OF THE MAMMALIAN CATALYTIC SUBUNIT OF CAMP-DEPENDENT PROTEIN KINASE AND AN INHIBITOR PEPTIDE DISPLAYS AN OPEN CONFORMATION
Authors	:	Karlsson, R.; Zheng, J.; Xuong, N.H.; Taylor, S.S.; Sowadski, J.M.
Deposited on	:	1993-04-08
Resolution	:	2.90 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 (1)) were used in the production of this report:

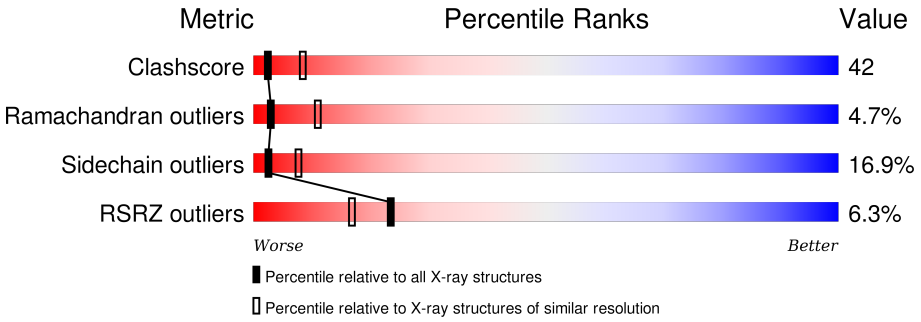
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	E	350	5% 28% 42% 18% 7% 5%
2	I	20	15% 15% 45% 10% 20% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2732 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.

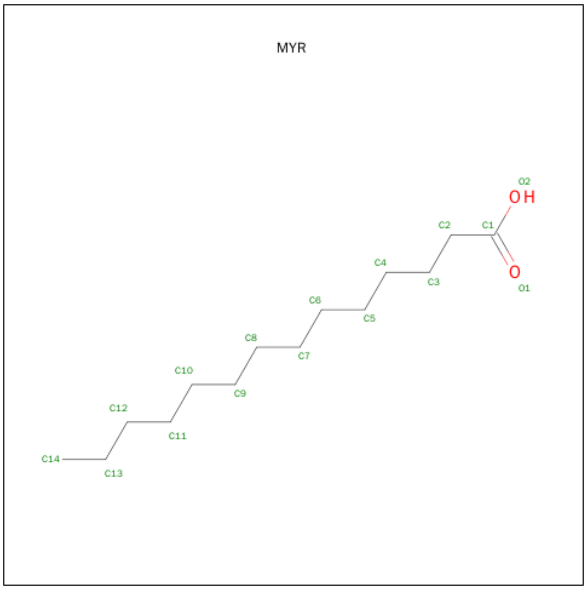
- Molecule 1 is a protein called cAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	333	Total	C	N	O	P	S	0	0	0
			2580	1679	431	461	1	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor, alpha form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	18	Total	C	I	N	O	0	0	0
			140	84	2	28	26			

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	C	0	0
			10	10		

- Molecule 4 is water.

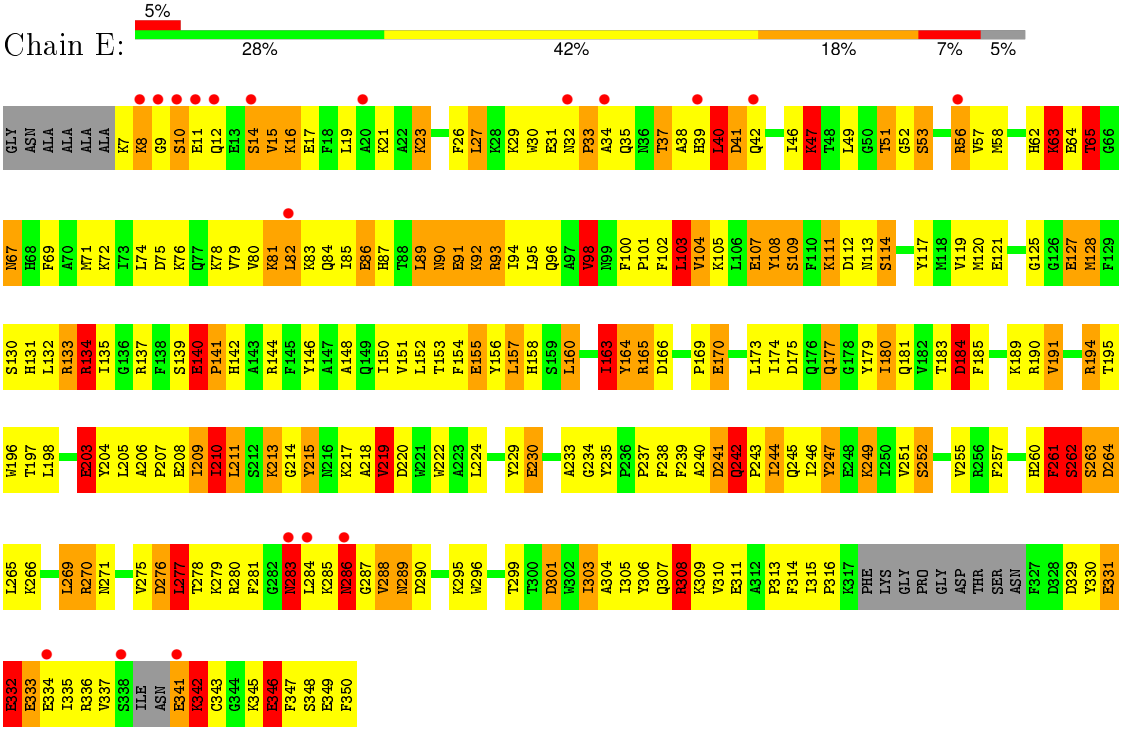
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total O 2 2	0	0

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.

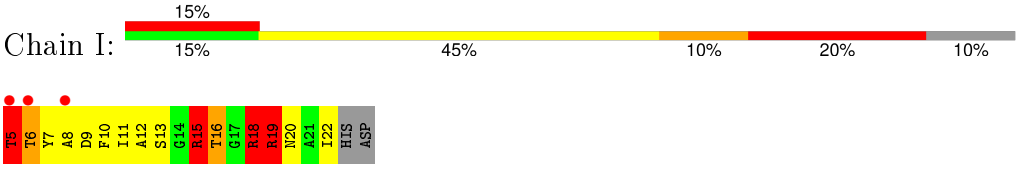
- Molecule 1: cAMP-DEPENDENT PROTEIN KINASE

Chain E:



- Molecule 2: cAMP-dependent protein kinase inhibitor, alpha form

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	171.50Å 171.50Å 171.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90 41.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.90) 99.0 (41.59-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.190 , (Not available) 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 19495 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2732	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MYR, TYI

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	1.32	16/2635 (0.6%)	2.33	123/3578 (3.4%)
2	I	1.23	0/125	2.81	16/165 (9.7%)
All	All	1.31	16/2760 (0.6%)	2.35	139/3743 (3.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	86	GLU	CD-OE2	13.63	1.40	1.25
1	E	349	GLU	CD-OE2	12.54	1.39	1.25
1	E	127	GLU	CD-OE2	9.90	1.36	1.25
1	E	121	GLU	CD-OE1	9.72	1.36	1.25
1	E	311	GLU	CD-OE1	9.12	1.35	1.25
1	E	91	GLU	CD-OE2	7.92	1.34	1.25
1	E	140	GLU	CD-OE1	7.03	1.33	1.25
1	E	332	GLU	CD-OE2	6.93	1.33	1.25
1	E	86	GLU	CD-OE1	5.81	1.32	1.25
1	E	346	GLU	CD-OE2	5.73	1.31	1.25
1	E	155	GLU	CD-OE1	5.59	1.31	1.25
1	E	208	GLU	CD-OE1	5.58	1.31	1.25
1	E	230	GLU	CD-OE1	-5.51	1.19	1.25
1	E	170	GLU	CD-OE1	-5.51	1.19	1.25
1	E	155	GLU	CD-OE2	-5.16	1.20	1.25
1	E	341	GLU	N-CA	5.05	1.56	1.46

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	194	ARG	NE-CZ-NH2	-17.45	111.58	120.30
1	E	280	ARG	NE-CZ-NH1	16.82	128.71	120.30
1	E	108	TYR	CB-CG-CD1	-14.93	112.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	108	TYR	CB-CG-CD2	13.07	128.84	121.00
1	E	280	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	E	194	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	E	184	ASP	CB-CG-OD1	-12.36	107.17	118.30
1	E	15	VAL	CA-CB-CG2	-12.15	92.68	110.90
1	E	137	ARG	NE-CZ-NH2	11.96	126.28	120.30
1	E	252	SER	CB-CA-C	-11.82	87.64	110.10
1	E	308	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	E	37	THR	CA-CB-CG2	-11.62	96.13	112.40
2	I	18	ARG	NE-CZ-NH1	-11.60	114.50	120.30
1	E	103	LEU	O-C-N	-10.47	105.94	122.70
1	E	277	LEU	CB-CG-CD2	-10.44	93.26	111.00
1	E	134	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	E	247	TYR	CB-CG-CD1	10.03	127.02	121.00
1	E	184	ASP	N-CA-CB	-9.71	93.12	110.60
1	E	98	VAL	CA-CB-CG2	-9.50	96.66	110.90
2	I	13	SER	C-N-CA	-9.15	103.08	122.30
1	E	308	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	E	56	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	E	262	SER	CB-CA-C	-8.69	93.59	110.10
1	E	330	TYR	CB-CG-CD2	8.56	126.13	121.00
1	E	34	ALA	CB-CA-C	8.50	122.85	110.10
1	E	177	GLN	N-CA-CB	-8.45	95.39	110.60
1	E	261	PHE	O-C-N	-8.44	109.20	122.70
1	E	247	TYR	CB-CG-CD2	-8.42	115.95	121.00
1	E	133	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	E	342	LYS	N-CA-CB	8.19	125.35	110.60
1	E	175	ASP	CB-CG-OD2	8.03	125.52	118.30
1	E	290	ASP	CB-CG-OD2	7.94	125.44	118.30
1	E	109	SER	N-CA-CB	-7.92	98.63	110.50
1	E	32	ASN	CB-CA-C	7.86	126.12	110.40
2	I	6	THR	CB-CA-C	-7.81	90.51	111.60
1	E	213	LYS	N-CA-CB	-7.73	96.69	110.60
1	E	288	VAL	CA-CB-CG2	-7.71	99.34	110.90
1	E	128	MET	CG-SD-CE	-7.68	87.91	100.20
1	E	277	LEU	CB-CA-C	-7.67	95.62	110.20
1	E	104	VAL	CA-CB-CG1	-7.65	99.43	110.90
1	E	67	ASN	CA-CB-CG	-7.57	96.75	113.40
1	E	164	TYR	C-N-CA	-7.56	102.80	121.70
1	E	93	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	E	134	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	I	9	ASP	CB-CA-C	-7.39	95.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	301	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	E	286	ASN	CB-CA-C	-7.34	95.73	110.40
1	E	133	ARG	CG-CD-NE	-7.32	96.43	111.80
2	I	5	THR	CA-CB-CG2	-7.20	102.33	112.40
1	E	89	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	E	137	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
1	E	343	CYS	CA-CB-SG	-6.98	101.44	114.00
1	E	164	TYR	O-C-N	-6.92	111.62	122.70
1	E	262	SER	N-CA-CB	-6.92	100.13	110.50
1	E	209	ILE	O-C-N	-6.64	112.07	122.70
1	E	163	ILE	CA-CB-CG1	6.63	123.61	111.00
1	E	237	PRO	O-C-N	-6.61	112.12	122.70
2	I	16	THR	CA-CB-OG1	-6.55	95.23	109.00
1	E	288	VAL	CG1-CB-CG2	-6.55	100.42	110.90
1	E	263	SER	N-CA-C	-6.54	93.33	111.00
1	E	341	GLU	CG-CD-OE2	6.53	131.35	118.30
1	E	41	ASP	N-CA-CB	-6.51	98.88	110.60
1	E	58	MET	CA-CB-CG	-6.50	102.26	113.30
1	E	262	SER	N-CA-C	-6.45	93.58	111.00
1	E	166	ASP	CB-CG-OD1	6.39	124.05	118.30
2	I	6	THR	CA-CB-CG2	-6.35	103.50	112.40
1	E	58	MET	CG-SD-CE	-6.31	90.11	100.20
1	E	289	ASN	CA-CB-CG	-6.29	99.57	113.40
1	E	238	PHE	CB-CG-CD1	-6.28	116.40	120.80
1	E	345	LYS	N-CA-CB	6.17	121.70	110.60
2	I	22	ILE	CA-CB-CG2	-6.10	98.70	110.90
1	E	63	LYS	O-C-N	-6.08	112.97	122.70
1	E	262	SER	CA-C-O	-6.07	107.35	120.10
1	E	166	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	E	219	VAL	CA-CB-CG2	6.05	119.97	110.90
1	E	313	PRO	N-CA-CB	5.98	110.47	103.30
1	E	348	SER	CA-CB-OG	-5.96	95.10	111.20
1	E	98	VAL	N-CA-CB	-5.96	98.39	111.50
1	E	134	ARG	CD-NE-CZ	5.93	131.91	123.60
1	E	342	LYS	CA-C-O	-5.92	107.68	120.10
1	E	121	GLU	CG-CD-OE1	-5.87	106.56	118.30
1	E	283	ASN	CB-CA-C	-5.86	98.67	110.40
2	I	15	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	10	SER	N-CA-CB	-5.83	101.76	110.50
1	E	72	LYS	CD-CE-NZ	5.82	125.09	111.70
1	E	331	GLU	N-CA-CB	-5.79	100.18	110.60
1	E	63	LYS	C-N-CA	-5.77	107.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	191	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	E	180	ILE	CB-CG1-CD1	-5.75	97.80	113.90
1	E	81	LYS	N-CA-CB	5.65	120.78	110.60
1	E	144	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	130	SER	CB-CA-C	-5.61	99.43	110.10
1	E	210	ILE	CB-CG1-CD1	-5.60	98.22	113.90
2	I	6	THR	N-CA-CB	-5.59	99.68	110.30
1	E	203	GLU	CG-CD-OE2	-5.55	107.21	118.30
1	E	270	ARG	N-CA-CB	5.55	120.58	110.60
1	E	286	ASN	CB-CG-ND2	-5.54	103.39	116.70
2	I	5	THR	C-N-CA	-5.54	107.86	121.70
1	E	156	TYR	CZ-CE2-CD2	-5.53	114.82	119.80
1	E	310	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	E	29	LYS	N-CA-CB	-5.47	100.75	110.60
1	E	303	ILE	CA-CB-CG1	-5.44	100.67	111.00
1	E	275	VAL	C-N-CA	-5.43	108.11	121.70
1	E	262	SER	CA-CB-OG	-5.43	96.54	111.20
1	E	107	GLU	CG-CD-OE1	5.42	129.13	118.30
1	E	180	ILE	CG1-CB-CG2	-5.40	99.53	111.40
1	E	16	LYS	CA-C-O	5.38	131.40	120.10
1	E	51	THR	C-N-CA	-5.36	111.05	122.30
1	E	333	GLU	C-N-CA	-5.32	108.39	121.70
1	E	301	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	107	GLU	CG-CD-OE2	-5.29	107.71	118.30
1	E	234	GLY	C-N-CA	5.29	134.93	121.70
1	E	270	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	184	ASP	OD1-CG-OD2	5.26	133.29	123.30
1	E	38	ALA	CB-CA-C	-5.25	102.23	110.10
1	E	329	ASP	O-C-N	-5.25	114.31	122.70
1	E	194	ARG	CD-NE-CZ	5.23	130.92	123.60
1	E	209	ILE	CA-C-O	5.23	131.07	120.10
1	E	141	PRO	N-CA-CB	5.22	109.56	103.30
2	I	20	ASN	CA-CB-CG	-5.22	101.92	113.40
2	I	19	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	41	ASP	C-N-CA	-5.20	108.70	121.70
2	I	15	ARG	CD-NE-CZ	-5.20	116.33	123.60
1	E	262	SER	O-C-N	5.19	131.01	122.70
1	E	164	TYR	N-CA-CB	-5.19	101.27	110.60
1	E	276	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	75	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	102	PHE	CB-CG-CD1	5.13	124.39	120.80
2	I	5	THR	CB-CA-C	-5.11	97.80	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	330	TYR	O-C-N	-5.08	114.57	122.70
1	E	166	ASP	N-CA-CB	-5.06	101.49	110.60
1	E	47	LYS	CB-CG-CD	-5.06	98.45	111.60
2	I	13	SER	O-C-N	-5.04	114.62	123.20
1	E	21	LYS	CB-CA-C	-5.04	100.32	110.40
1	E	215	TYR	CB-CG-CD1	5.03	124.02	121.00
1	E	241	ASP	CA-C-O	-5.03	109.55	120.10
1	E	264	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	E	233	ALA	N-CA-CB	5.01	117.12	110.10
1	E	242	GLN	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

There are no planarity outliers.

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	E	2580	0	2409	208	1
2	I	140	0	132	22	0
3	E	10	0	19	0	0
4	E	2	0	0	0	0
All	All	2732	0	2560	223	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 42.

All (223) 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:15:VAL:HG23	1:E:16:LYS:N	1.61	1.10
1:E:65:THR:HG22	1:E:67:ASN:H	1.14	1.10
2:I:11:ILE:C	2:I:11:ILE:HD12	1.78	1.04
1:E:23:LYS:HD2	1:E:27:LEU:HD22	1.36	1.03
1:E:284:LEU:N	1:E:284:LEU:HD12	1.75	0.99
1:E:15:VAL:CG2	1:E:16:LYS:N	2.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:LYS:HD2	1:E:27:LEU:CD2	1.98	0.94
1:E:140:GLU:HB3	1:E:141:PRO:HD3	1.50	0.94
1:E:346:GLU:OE1	1:E:346:GLU:N	2.03	0.91
1:E:284:LEU:H	1:E:284:LEU:CD1	1.84	0.90
1:E:301:ASP:HB3	1:E:304:ALA:HB3	1.54	0.90
1:E:31:GLU:O	1:E:33:PRO:HD3	1.73	0.89
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.08	0.88
1:E:64:GLU:O	1:E:65:THR:HB	1.74	0.88
1:E:39:HIS:O	1:E:42:GLN:HG2	1.74	0.87
1:E:189:LYS:HD3	1:E:191:VAL:HG11	1.55	0.87
1:E:284:LEU:N	1:E:284:LEU:CD1	2.37	0.87
1:E:140:GLU:OE2	1:E:262:SER:OG	1.95	0.84
1:E:65:THR:CG2	1:E:67:ASN:HB2	2.10	0.82
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.63	0.81
1:E:198:LEU:HD12	1:E:209:ILE:HG22	1.62	0.80
1:E:31:GLU:C	1:E:33:PRO:HD3	2.03	0.80
1:E:37:THR:HG21	1:E:108:TYR:HD1	1.43	0.80
2:I:11:ILE:O	2:I:11:ILE:HD12	1.81	0.79
1:E:184:ASP:OD1	1:E:184:ASP:C	2.19	0.79
1:E:194:ARG:NH2	1:E:213:LYS:O	2.16	0.78
1:E:205:LEU:HD12	1:E:247:TYR:HE1	1.47	0.78
1:E:153:THR:HG22	1:E:157:LEU:HD22	1.66	0.77
2:I:11:ILE:C	2:I:11:ILE:CD1	2.53	0.77
1:E:15:VAL:CG2	1:E:16:LYS:H	1.96	0.76
1:E:84:GLN:NE2	1:E:87:HIS:HD2	1.84	0.76
1:E:205:LEU:HD12	1:E:247:TYR:CE1	2.21	0.76
2:I:6:THR:HG22	2:I:7:TYI:N	1.99	0.75
1:E:65:THR:CG2	1:E:67:ASN:H	1.98	0.75
1:E:65:THR:HG22	1:E:67:ASN:N	1.99	0.74
1:E:15:VAL:HG23	1:E:16:LYS:H	1.52	0.74
1:E:170:GLU:OE2	2:I:19:ARG:HD2	1.86	0.74
1:E:303:ILE:O	1:E:307:GLN:HG3	1.87	0.74
1:E:69:PHE:CE2	1:E:107:GLU:HG2	2.23	0.73
1:E:7:LYS:O	1:E:8:LYS:C	2.27	0.72
1:E:23:LYS:O	1:E:23:LYS:HG3	1.80	0.72
1:E:203:GLU:OE2	2:I:15:ARG:NH2	2.20	0.71
1:E:7:LYS:N	1:E:10:SER:HB3	2.06	0.70
1:E:245:GLN:O	1:E:249:LYS:HD2	1.92	0.70
1:E:197:TPO:HG23	1:E:198:LEU:N	2.06	0.70
2:I:11:ILE:O	2:I:11:ILE:CD1	2.39	0.70
1:E:7:LYS:O	1:E:10:SER:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:THR:HG21	1:E:108:TYR:CD1	2.26	0.68
1:E:131:HIS:O	1:E:135:ILE:HG13	1.93	0.68
1:E:27:LEU:HD11	1:E:190:ARG:NH2	2.09	0.67
1:E:262:SER:HB2	1:E:265:LEU:HB3	1.76	0.67
1:E:65:THR:HG23	1:E:67:ASN:HB2	1.76	0.67
1:E:76:LYS:HB3	1:E:347:PHE:CE2	2.29	0.67
1:E:189:LYS:HG2	1:E:191:VAL:HG12	1.77	0.66
1:E:40:LEU:O	1:E:42:GLN:N	2.28	0.66
1:E:104:VAL:O	1:E:104:VAL:HG13	1.96	0.65
1:E:230:GLU:CD	2:I:19:ARG:HH22	2.00	0.65
1:E:211:LEU:HD22	1:E:251:VAL:HG22	1.79	0.64
1:E:286:ASN:O	1:E:287:GLY:C	2.35	0.63
1:E:152:LEU:O	1:E:155:GLU:HB3	1.98	0.63
1:E:284:LEU:H	1:E:284:LEU:HD13	1.64	0.63
1:E:112:ASP:C	1:E:112:ASP:OD1	2.36	0.62
1:E:51:THR:HA	1:E:56:ARG:HA	1.82	0.62
1:E:243:PRO:O	1:E:244:ILE:C	2.37	0.61
1:E:100:PHE:CD1	1:E:101:PRO:HD2	2.34	0.61
1:E:100:PHE:CD2	1:E:101:PRO:HD2	2.36	0.61
1:E:194:ARG:HH21	1:E:214:GLY:HA3	1.66	0.61
1:E:197:TPO:CG2	1:E:198:LEU:N	2.63	0.61
1:E:84:GLN:HE22	1:E:87:HIS:HD2	1.48	0.61
1:E:78:LYS:O	1:E:82:LEU:HD12	2.01	0.60
1:E:183:THR:O	1:E:184:ASP:HB3	2.00	0.60
1:E:101:PRO:HG3	1:E:306:TYR:CE1	2.36	0.60
1:E:257:PHE:HE1	1:E:269:LEU:HD23	1.67	0.59
1:E:307:GLN:O	1:E:308:ARG:C	2.35	0.59
1:E:103:LEU:O	1:E:104:VAL:C	2.30	0.59
1:E:128:MET:HE2	1:E:169:PRO:HB3	1.84	0.59
1:E:7:LYS:O	1:E:10:SER:N	2.36	0.59
1:E:301:ASP:HB3	1:E:304:ALA:CB	2.31	0.59
1:E:180:ILE:C	1:E:180:ILE:HD12	2.23	0.59
1:E:128:MET:CE	1:E:169:PRO:HB3	2.33	0.58
2:I:6:THR:CG2	2:I:7:TYI:N	2.62	0.58
1:E:189:LYS:CD	1:E:191:VAL:HG11	2.30	0.58
1:E:112:ASP:OD1	1:E:114:SER:N	2.34	0.58
1:E:341:GLU:HG3	1:E:342:LYS:H	1.68	0.58
1:E:179:TYR:CZ	1:E:308:ARG:HA	2.39	0.57
1:E:131:HIS:HA	1:E:134:ARG:HH11	1.69	0.57
1:E:257:PHE:CE1	1:E:269:LEU:HD23	2.40	0.57
2:I:5:THR:O	2:I:5:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:GLU:HB3	1:E:141:PRO:CD	2.32	0.56
2:I:18:ARG:CB	2:I:18:ARG:HH11	2.18	0.56
1:E:163:ILE:HG12	1:E:165:ARG:HD3	1.87	0.55
1:E:133:ARG:HD2	2:I:16:THR:O	2.05	0.55
1:E:189:LYS:HE2	1:E:195:THR:OG1	2.06	0.55
1:E:83:LYS:C	1:E:84:GLN:HG2	2.26	0.55
1:E:285:LYS:O	1:E:286:ASN:CG	2.46	0.55
1:E:262:SER:CB	1:E:265:LEU:H	2.20	0.54
1:E:98:VAL:HG13	1:E:103:LEU:HD23	1.88	0.54
1:E:16:LYS:O	1:E:17:GLU:C	2.43	0.54
1:E:239:PHE:CZ	2:I:10:PHE:HB2	2.42	0.54
1:E:98:VAL:CG1	1:E:103:LEU:HD23	2.37	0.54
1:E:30:TRP:O	1:E:93:ARG:NH2	2.41	0.54
1:E:15:VAL:HG22	1:E:16:LYS:H	1.70	0.54
1:E:52:GLY:C	1:E:53:SER:O	2.45	0.53
1:E:164:TYR:O	1:E:220:ASP:OD1	2.27	0.53
1:E:78:LYS:O	1:E:82:LEU:CD1	2.57	0.53
1:E:12:GLN:O	1:E:15:VAL:HG22	2.09	0.52
1:E:93:ARG:O	1:E:96:GLN:NE2	2.34	0.52
1:E:84:GLN:HE22	1:E:87:HIS:CD2	2.28	0.52
1:E:230:GLU:OE1	2:I:19:ARG:NH2	2.42	0.52
1:E:276:ASP:O	1:E:278:THR:N	2.43	0.52
1:E:101:PRO:CG	1:E:306:TYR:CE1	2.93	0.52
1:E:104:VAL:O	1:E:104:VAL:CG1	2.58	0.52
1:E:206:ALA:O	1:E:207:PRO:C	2.48	0.52
1:E:334:GLU:O	1:E:335:ILE:C	2.48	0.52
1:E:154:PHE:CE2	1:E:220:ASP:HB3	2.45	0.52
2:I:6:THR:HG22	2:I:8:ALA:H	1.75	0.51
1:E:241:ASP:O	1:E:242:GLN:CB	2.58	0.51
1:E:23:LYS:CD	1:E:27:LEU:HD22	2.24	0.51
1:E:62:HIS:CD2	1:E:65:THR:HB	2.47	0.50
1:E:112:ASP:O	1:E:113:ASN:C	2.47	0.50
1:E:217:LYS:O	1:E:218:ALA:C	2.49	0.50
1:E:210:ILE:HD12	1:E:247:TYR:HB3	1.92	0.50
1:E:76:LYS:HE3	1:E:113:ASN:O	2.11	0.50
1:E:263:SER:O	1:E:266:LYS:N	2.45	0.50
1:E:206:ALA:HB1	1:E:207:PRO:HD2	1.92	0.50
1:E:8:LYS:O	1:E:11:GLU:N	2.44	0.50
1:E:276:ASP:O	1:E:279:LYS:N	2.30	0.50
1:E:142:HIS:NE2	1:E:146:TYR:CE2	2.80	0.50
1:E:85:ILE:HG22	1:E:89:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:THR:N	1:E:215:TYR:O	2.45	0.49
1:E:307:GLN:HB2	1:E:309:LYS:HD2	1.94	0.49
2:I:18:ARG:CB	2:I:18:ARG:NH1	2.75	0.49
2:I:5:THR:O	2:I:6:THR:OG1	2.26	0.49
1:E:180:ILE:HD12	1:E:181:GLN:N	2.28	0.48
1:E:91:GLU:HG3	1:E:185:PHE:HB2	1.94	0.48
1:E:262:SER:HB2	1:E:265:LEU:H	1.77	0.48
1:E:209:ILE:HD11	1:E:219:VAL:HG11	1.96	0.48
1:E:314:PHE:O	1:E:315:ILE:HG12	2.14	0.48
1:E:206:ALA:HB3	1:E:219:VAL:HG12	1.95	0.48
1:E:46:ILE:O	1:E:47:LYS:CB	2.59	0.48
1:E:271:ASN:HB3	1:E:281:PHE:CD1	2.49	0.48
1:E:260:HIS:O	1:E:261:PHE:O	2.32	0.48
1:E:346:GLU:H	1:E:346:GLU:CD	2.16	0.48
1:E:37:THR:CG2	1:E:108:TYR:HD1	2.20	0.48
2:I:18:ARG:HB3	2:I:18:ARG:NH1	2.29	0.48
1:E:169:PRO:HD3	1:E:204:TYR:OH	2.14	0.47
1:E:160:LEU:O	1:E:190:ARG:HD2	2.14	0.47
1:E:83:LYS:O	1:E:84:GLN:HG2	2.13	0.47
1:E:82:LEU:O	1:E:84:GLN:HG2	2.14	0.47
1:E:205:LEU:CD1	1:E:247:TYR:CE1	2.95	0.47
1:E:14:SER:O	1:E:15:VAL:C	2.52	0.47
1:E:239:PHE:O	1:E:240:ALA:HB2	2.15	0.47
1:E:229:TYR:C	1:E:229:TYR:CD1	2.88	0.47
1:E:189:LYS:CG	1:E:191:VAL:HG12	2.44	0.47
1:E:15:VAL:O	1:E:16:LYS:C	2.53	0.46
2:I:11:ILE:HG13	2:I:11:ILE:H	1.62	0.46
1:E:127:GLU:HA	1:E:173:LEU:HA	1.97	0.46
1:E:46:ILE:O	1:E:47:LYS:HB3	2.14	0.46
1:E:40:LEU:HD23	1:E:40:LEU:HA	1.74	0.46
1:E:203:GLU:H	1:E:203:GLU:HG2	1.21	0.46
1:E:194:ARG:HA	1:E:215:TYR:O	2.15	0.46
1:E:100:PHE:CG	1:E:101:PRO:CD	2.91	0.46
1:E:125:GLY:HA3	1:E:316:PRO:HG2	1.97	0.46
2:I:11:ILE:HD12	2:I:12:ALA:N	2.25	0.45
1:E:105:LYS:O	1:E:120:MET:HG3	2.16	0.45
1:E:84:GLN:HE21	1:E:84:GLN:HA	1.81	0.45
1:E:184:ASP:OD1	1:E:184:ASP:O	2.34	0.45
2:I:5:THR:C	2:I:6:THR:OG1	2.54	0.45
1:E:307:GLN:O	1:E:309:LYS:N	2.49	0.45
1:E:19:LEU:HA	1:E:19:LEU:HD23	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ASN:O	1:E:289:ASN:HB2	2.17	0.45
1:E:210:ILE:HG21	1:E:210:ILE:HD13	1.24	0.45
1:E:174:ILE:CD1	1:E:180:ILE:HG22	2.47	0.45
1:E:239:PHE:C	1:E:239:PHE:CD1	2.90	0.45
1:E:111:LYS:HE2	1:E:350:PHE:O	2.17	0.45
1:E:109:SER:HA	1:E:117:TYR:O	2.17	0.44
1:E:189:LYS:CD	1:E:191:VAL:CG1	2.95	0.44
1:E:189:LYS:CG	1:E:191:VAL:CG1	2.96	0.44
1:E:69:PHE:HB3	1:E:120:MET:O	2.17	0.44
1:E:91:GLU:HG3	1:E:185:PHE:CB	2.48	0.44
1:E:135:ILE:HG22	1:E:135:ILE:O	2.18	0.44
1:E:243:PRO:O	1:E:246:ILE:N	2.49	0.44
1:E:31:GLU:O	1:E:33:PRO:CD	2.56	0.43
1:E:307:GLN:C	1:E:309:LYS:N	2.70	0.43
1:E:266:LYS:O	1:E:270:ARG:HG2	2.18	0.43
1:E:277:LEU:HA	1:E:277:LEU:HD23	1.08	0.43
1:E:240:ALA:HB2	1:E:249:LYS:HE3	1.99	0.43
1:E:26:PHE:CG	1:E:160:LEU:HG	2.53	0.43
1:E:92:LYS:HG3	1:E:350:PHE:CE2	2.53	0.43
1:E:139:SER:O	1:E:140:GLU:C	2.57	0.43
1:E:84:GLN:NE2	1:E:87:HIS:CD2	2.73	0.43
1:E:71:MET:HG3	1:E:119:VAL:HG22	2.01	0.43
1:E:241:ASP:O	1:E:245:GLN:NE2	2.52	0.43
1:E:150:ILE:O	1:E:151:VAL:C	2.55	0.43
1:E:9:GLY:O	1:E:10:SER:C	2.56	0.42
1:E:158:HIS:CE1	1:E:220:ASP:OD2	2.55	0.42
1:E:271:ASN:HB3	1:E:281:PHE:CG	2.54	0.42
1:E:63:LYS:HG2	1:E:63:LYS:H	1.68	0.42
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.48	0.42
1:E:269:LEU:HA	1:E:269:LEU:HD12	1.89	0.42
1:E:165:ARG:NH1	1:E:215:TYR:OH	2.53	0.42
1:E:179:TYR:CE2	1:E:308:ARG:HA	2.55	0.42
1:E:235:TYR:CD1	1:E:235:TYR:N	2.87	0.42
1:E:195:THR:O	1:E:214:GLY:HA2	2.19	0.41
1:E:249:LYS:HG2	1:E:249:LYS:HZ2	1.59	0.41
1:E:80:VAL:O	1:E:81:LYS:C	2.59	0.41
1:E:26:PHE:O	1:E:27:LEU:C	2.58	0.41
1:E:283:ASN:HD22	1:E:283:ASN:HA	1.59	0.41
1:E:95:LEU:HD23	1:E:95:LEU:HA	1.81	0.41
1:E:303:ILE:HG13	1:E:303:ILE:H	1.73	0.41
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LEU:O	1:E:133:ARG:C	2.59	0.41
1:E:262:SER:HB3	1:E:265:LEU:H	1.85	0.41
1:E:295:LYS:O	1:E:296:TRP:C	2.59	0.41
1:E:288:VAL:H	1:E:288:VAL:HG23	1.71	0.41
1:E:169:PRO:HD2	2:I:19:ARG:HH12	1.86	0.41
1:E:334:GLU:O	1:E:336:ARG:N	2.54	0.41
1:E:270:ARG:HH11	1:E:270:ARG:HD2	1.77	0.41
1:E:331:GLU:O	1:E:332:GLU:O	2.39	0.41
1:E:100:PHE:O	1:E:101:PRO:C	2.58	0.40
1:E:49:LEU:HB2	1:E:57:VAL:O	2.21	0.40
1:E:90:ASN:O	1:E:94:ILE:HG13	2.21	0.40
1:E:148:ALA:HB3	1:E:305:ILE:HD12	2.03	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)
1:E:86:GLU:OE2	1:E:196:TRP:CZ3[24_555]	2.10	0.10

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	E	326/350 (93%)	272 (83%)	38 (12%)	16 (5%)	3 10
2	I	15/20 (75%)	12 (80%)	3 (20%)	0	100 100
All	All	341/370 (92%)	284 (83%)	41 (12%)	16 (5%)	3 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	33	PRO

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Mol	Chain	Res	Type
1	E	41	ASP
1	E	242	GLN
1	E	332	GLU
1	E	337	VAL
1	E	342	LYS
1	E	8	LYS
1	E	40	LEU
1	E	65	THR
1	E	277	LEU
1	E	286	ASN
1	E	184	ASP
1	E	261	PHE
1	E	264	ASP
1	E	244	ILE
1	E	333	GLU

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	E	249/304 (82%)	209 (84%)	40 (16%)	3 9
2	I	12/14 (86%)	8 (67%)	4 (33%)	0 1
All	All	261/318 (82%)	217 (83%)	44 (17%)	2 8

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	14	SER
1	E	23	LYS
1	E	27	LEU
1	E	35	GLN
1	E	40	LEU
1	E	47	LYS
1	E	53	SER
1	E	63	LYS

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Mol	Chain	Res	Type
1	E	65	THR
1	E	74	LEU
1	E	79	VAL
1	E	82	LEU
1	E	90	ASN
1	E	92	LYS
1	E	98	VAL
1	E	103	LEU
1	E	111	LYS
1	E	114	SER
1	E	134	ARG
1	E	140	GLU
1	E	157	LEU
1	E	160	LEU
1	E	163	ILE
1	E	165	ARG
1	E	177	GLN
1	E	203	GLU
1	E	210	ILE
1	E	211	LEU
1	E	219	VAL
1	E	222	TRP
1	E	224	LEU
1	E	249	LYS
1	E	252	SER
1	E	255	VAL
1	E	262	SER
1	E	269	LEU
1	E	283	ASN
1	E	299	THR
1	E	308	ARG
1	E	346	GLU
2	I	5	THR
2	I	15	ARG
2	I	18	ARG
2	I	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	GLN
1	E	62	HIS

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Mol	Chain	Res	Type
1	E	84	GLN
1	E	87	HIS
1	E	158	HIS
1	E	245	GLN
1	E	271	ASN
1	E	283	ASN
1	E	289	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	TPO	E	197	1	8,10,11	1.26	1 (12%)	7,14,16	2.52	3 (42%)
2	TYI	I	7	2	13,14,15	1.89	1 (7%)	16,19,21	3.00	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
1	TPO	E	197	1	-	0/8/11/13	0/0/0/0
2	TYI	I	7	2	-	0/4/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	7	TYI	CE1-I1	-6.17	1.93	2.10
1	E	197	TPO	P-OG1	-2.23	1.53	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	7	TYI	CD1-CE1-I1	-7.12	105.10	118.60
1	E	197	TPO	CG2-CB-CA	-4.66	103.68	113.17
2	I	7	TYI	CB-CG-CD2	-4.39	111.88	120.36
2	I	7	TYI	CG-CB-CA	-3.61	106.06	114.21
2	I	7	TYI	CD2-CE2-I2	-3.15	112.62	118.60
2	I	7	TYI	CG-CD2-CE2	-2.19	115.60	120.36
2	I	7	TYI	CD1-CE1-CZ	-2.06	116.36	121.00
1	E	197	TPO	OG1-P-O1P	2.53	113.43	107.11
2	I	7	TYI	CD2-CE2-CZ	2.75	127.21	121.00
1	E	197	TPO	C-CA-N	3.75	117.67	109.83
2	I	7	TYI	CB-CG-CD1	4.65	129.33	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	197	TPO	2	0
2	I	7	TYI	2	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	MYR	E	0	-	9,9,15	0.51	0	8,8,15	0.71	0

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	MYR	E	0	-	-	0/7/7/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	E	332/350 (94%)	0.23	19 (5%) 27 21	16, 20, 30, 40	0
2	I	17/20 (85%)	0.99	3 (17%) 2 1	16, 22, 30, 31	0
All	All	349/370 (94%)	0.27	22 (6%) 23 17	16, 20, 30, 40	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	5	THR	5.7
2	I	6	THR	4.6
1	E	10	SER	4.6
1	E	9	GLY	4.4
1	E	283	ASN	4.1
1	E	341	GLU	3.7
1	E	11	GLU	3.6
1	E	39	HIS	3.3
1	E	42	GLN	3.2
1	E	14	SER	3.0
1	E	82	LEU	2.9
1	E	284	LEU	2.9
1	E	338	SER	2.8
2	I	8	ALA	2.5
1	E	32	ASN	2.3
1	E	12	GLN	2.3
1	E	8	LYS	2.2
1	E	56	ARG	2.2
1	E	286	ASN	2.2
1	E	20	ALA	2.1
1	E	334	GLU	2.1
1	E	34	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TYI	I	7	14/15	0.98	0.19	-	16,25,33,35	0
1	TPO	E	197	11/12	0.94	0.20	-	16,18,25,28	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MYR	E	0	10/16	0.96	0.14	-1.11	16,16,28,30	0

6.5 Other polymers (i)

There are no such residues in this entry.