



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 01:31 am GMT

PDB ID : 2WHB  
Title : Truncation and Optimisation of Peptide Inhibitors of CDK2, Cyclin A Through Structure Guided Design  
Authors : Kontopidis, G.; Andrews, M.J.; McInnes, C.; Plater, A.; Innes, L.; Renachowski, S.; Cowan, A.; Fischer, P.M.  
Deposited on : 2009-05-03  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

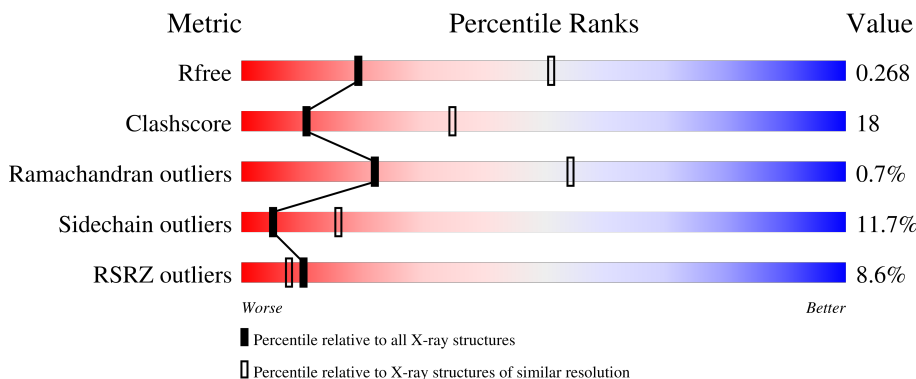
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.



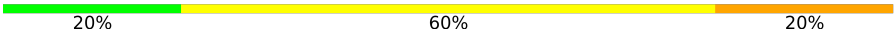
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	298	 10% 54% 34% 10% ..
1	C	298	 11% 60% 32% 7% .
2	B	260	 5% 62% 31% 6% .
2	D	260	 8% 62% 32% 6% .
3	E	5	 20% 60% 20%

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Mol	Chain	Length	Quality of chain
3	F	5	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9125 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	Total 2378	C 1547	N 403	O 420	S 8	0	0	0
1	C	297	Total 2379	C 1547	N 404	O 420	S 8	0	0	1

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	Total 2094	C 1358	N 341	O 384	S 11	0	2	0
2	D	258	Total 2084	C 1350	N 339	O 384	S 11	0	0	0

- Molecule 3 is a protein called ARG-ARG-L3O-PFF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
3	E	5	Total 45	C 28	F 1	N 11	O 5	0	0	1
3	F	5	Total 45	C 28	F 1	N 11	O 5	0	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total 26 O 26	0	0
4	B	18	Total 18 O 18	0	0
4	C	37	Total 37 O 37	0	0
4	D	17	Total 17 O 17	0	0

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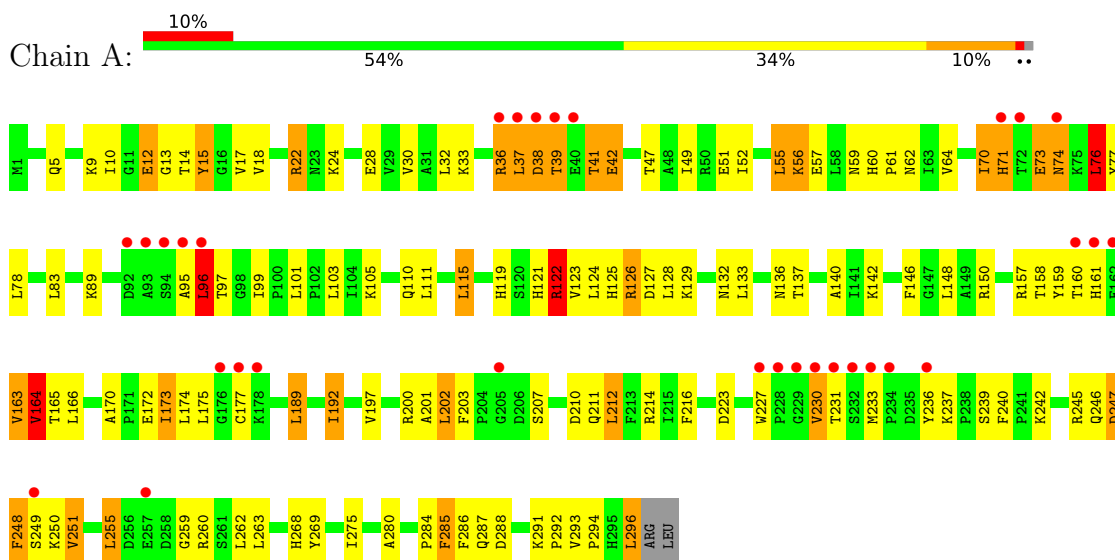
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	F	2	Total	O	0	0
			2	2		

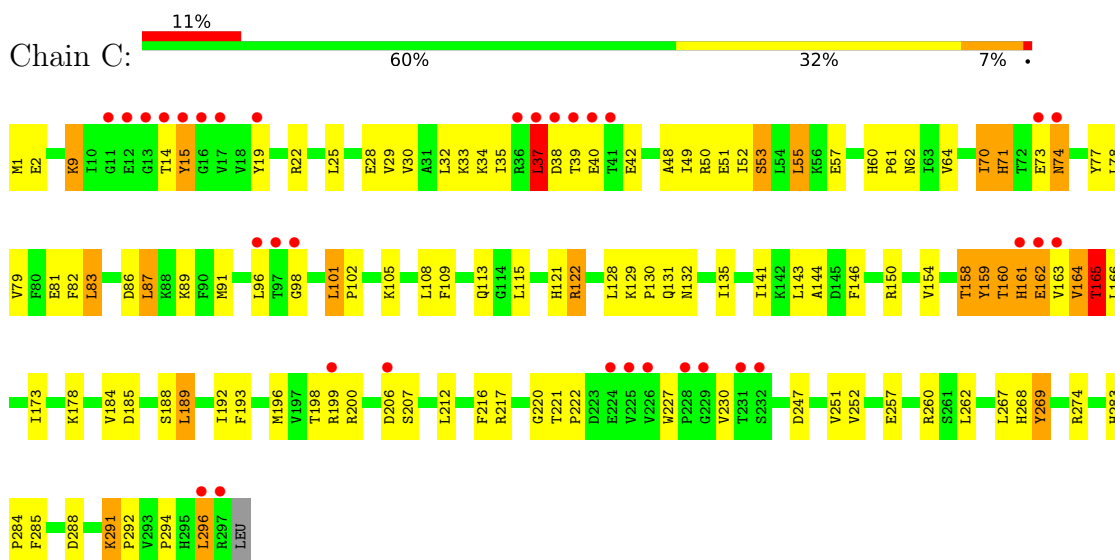
### 3 Residue-property plots

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

- Molecule 1: CELL DIVISION PROTEIN KINASE 2

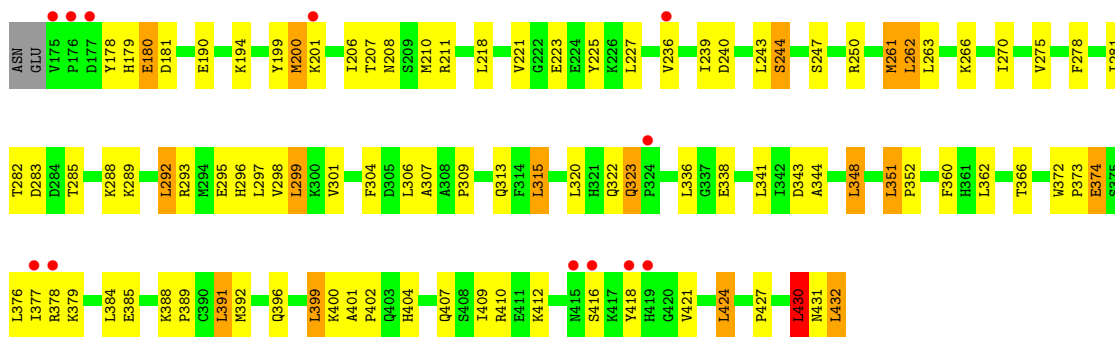


- Molecule 1: CELL DIVISION PROTEIN KINASE 2

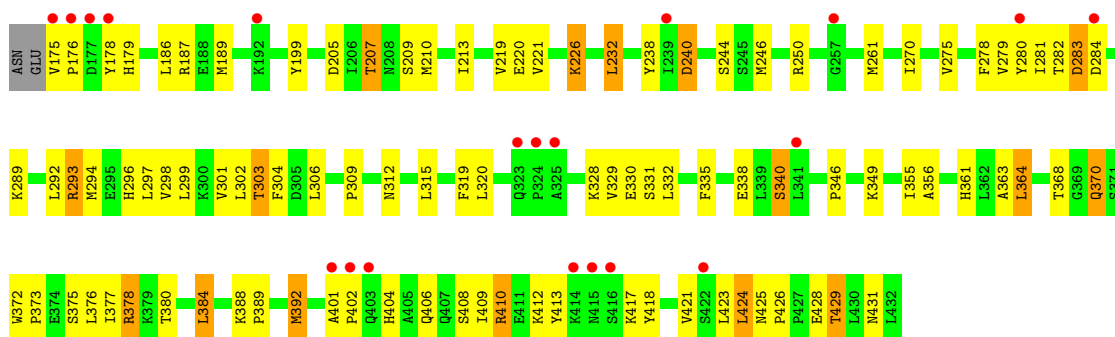


- Molecule 2: CYCLIN-A2

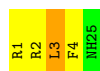
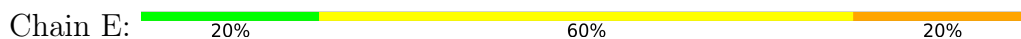




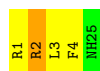
• Molecule 2: CYCLIN-A2



• Molecule 3: ARG-ARG-L3O-PFF



• Molecule 3: ARG-ARG-L3O-PFF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.42Å 114.92Å 154.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.90) 97.4 (29.83-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.264 0.193 , 0.268	Depositor DCC
$R_{free}$ test set	944 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PFF, L3O, NH2

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	0.65	0/2440	1.37	22/3313 (0.7%)
1	C	0.64	2/2441 (0.1%)	1.36	20/3315 (0.6%)
2	B	0.60	0/2150	1.34	20/2920 (0.7%)
2	D	0.60	0/2134	1.34	12/2897 (0.4%)
3	E	0.51	0/21	3.05	2/25 (8.0%)
3	F	0.72	0/21	2.88	2/25 (8.0%)
All	All	0.62	2/9207 (0.0%)	1.36	78/12495 (0.6%)

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	1
3	E	0	2
3	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	TYR	CE2-CZ	5.27	1.45	1.38
1	C	162	GLU	CB-CG	5.05	1.61	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	240	ASP	CB-CG-OD1	-13.27	106.36	118.30
2	D	240	ASP	CB-CG-OD2	10.84	128.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	ARG	NE-CZ-NH1	-9.91	115.34	120.30
3	E	1	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	223	ASP	CB-CG-OD2	9.80	127.12	118.30
1	A	127	ASP	CB-CG-OD1	9.52	126.87	118.30
1	C	83	LEU	CB-CG-CD1	-9.28	95.22	111.00
2	B	424	LEU	CB-CG-CD2	-9.09	95.55	111.00
1	C	185	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	200	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	127	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	247	ASP	CB-CG-OD2	8.39	125.86	118.30
1	A	189	LEU	CB-CG-CD2	-8.22	97.03	111.00
1	C	260	ARG	NE-CZ-NH2	-8.11	116.24	120.30
3	F	1	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	C	288	ASP	CB-CG-OD2	-7.76	111.32	118.30
2	D	423	LEU	CB-CG-CD2	-7.69	97.92	111.00
1	C	150	ARG	NE-CZ-NH2	-7.19	116.70	120.30
2	B	391	LEU	CB-CG-CD2	-7.07	98.98	111.00
2	B	424	LEU	CB-CG-CD1	7.02	122.94	111.00
1	A	173	ILE	CG1-CB-CG2	-7.02	95.95	111.40
2	B	378	ARG	NE-CZ-NH1	6.91	123.76	120.30
3	F	2	ARG	NE-CZ-NH2	-6.87	116.87	120.30
2	B	315	LEU	CB-CG-CD2	-6.74	99.54	111.00
2	B	194	LYS	CD-CE-NZ	6.73	127.18	111.70
2	B	299	LEU	CB-CG-CD2	-6.70	99.61	111.00
2	D	392	MET	CG-SD-CE	6.66	110.85	100.20
2	D	378	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	57	GLU	OE1-CD-OE2	-6.50	115.49	123.30
2	B	378	ARG	NE-CZ-NH2	-6.49	117.06	120.30
2	D	187	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	301	VAL	CG1-CB-CG2	6.25	120.90	110.90
1	C	267	LEU	CB-CG-CD2	-6.23	100.40	111.00
1	C	122	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	260	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	B	410	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	274	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	76	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	22	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	37	LEU	CA-CB-CG	-5.88	101.78	115.30
1	A	200	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	D	261	MET	CG-SD-CE	5.86	109.57	100.20
1	C	22	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	160	THR	CA-CB-CG2	-5.81	104.26	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	424	LEU	CB-CG-CD1	5.81	120.88	111.00
1	C	206	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	158	THR	CA-CB-CG2	-5.74	104.36	112.40
1	A	150	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	32	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	A	124	LEU	CB-CA-C	-5.68	99.41	110.20
2	D	205	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	298	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	A	18	VAL	CG1-CB-CG2	-5.60	101.94	110.90
2	D	246	MET	CG-SD-CE	5.57	109.11	100.20
1	C	101	LEU	CB-CG-CD2	5.53	120.40	111.00
2	B	384	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	C	162	GLU	OE1-CD-OE2	5.47	129.87	123.30
2	B	430	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	B	181	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	201	ALA	CB-CA-C	5.42	118.22	110.10
1	C	38	ASP	CB-CG-OD1	-5.41	113.43	118.30
2	B	211	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	E	1	ARG	NH1-CZ-NH2	5.39	125.33	119.40
2	D	410	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	257	GLU	OE1-CD-OE2	5.31	129.68	123.30
2	D	275	VAL	CA-CB-CG1	-5.25	103.03	110.90
1	C	262	LEU	CB-CG-CD2	-5.24	102.09	111.00
2	B	181	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	96	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	122	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	42	GLU	OE1-CD-OE2	-5.15	117.11	123.30
2	B	351	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	12	GLU	N-CA-CB	5.12	119.81	110.60
2	B	399	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	B	262	LEU	CB-CG-CD1	5.07	119.61	111.00
2	B	261	MET	CG-SD-CE	-5.03	92.15	100.20
1	C	29	VAL	CG1-CB-CG2	5.01	118.91	110.90
1	A	122	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	VAL	Peptide
3	E	3	L3O	Mainchain,Peptide
3	F	3	L3O	Mainchain,Peptide

## 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	2378	0	2426	118	0
1	C	2379	0	2426	86	0
2	B	2094	0	2123	81	0
2	D	2084	0	2107	66	0
3	E	45	0	47	0	0
3	F	45	0	47	0	0
4	A	26	0	0	0	0
4	B	18	0	0	0	0
4	C	37	0	0	0	0
4	D	17	0	0	1	0
4	F	2	0	0	0	0
All	All	9125	0	9176	333	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 18.

All (333) 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:A:38:ASP:CB	1:A:41:THR:HB	1.73	1.17
2:B:207:THR:HG22	2:B:210:MET:HG3	1.34	1.08
2:D:207:THR:HG22	2:D:210:MET:HG3	1.38	1.03
1:A:38:ASP:HB2	1:A:41:THR:HB	1.07	1.03
1:C:135:ILE:HG22	1:C:141:ILE:HG13	1.40	1.00
2:D:209:SER:O	2:D:213:ILE:HD12	1.63	0.97
1:A:163:VAL:HG13	1:A:163:VAL:O	1.70	0.92
2:B:282:THR:O	2:B:285:THR:HG22	1.70	0.90
1:A:137:THR:HG22	1:A:296:LEU:HD23	1.52	0.90
1:C:15:TYR:C	1:C:15:TYR:HD2	1.75	0.88
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.73	0.88
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.42	0.87
1:A:71:HIS:ND1	1:A:76:LEU:HD23	1.90	0.87
1:C:83:LEU:N	1:C:83:LEU:HD12	1.90	0.86
2:B:266:LYS:NZ	2:B:295:GLU:OE2	2.09	0.85
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:HIS:HE1	2:D:384:LEU:HD21	1.41	0.84
2:B:179:HIS:NE2	2:B:379:LYS:NZ	2.23	0.84
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.13	0.84
1:C:15:TYR:C	1:C:15:TYR:CD2	2.51	0.83
2:D:404:HIS:NE2	2:D:406:GLN:OE1	2.11	0.83
2:B:282:THR:HB	2:B:285:THR:CG2	2.09	0.82
1:A:71:HIS:NE2	2:B:296:HIS:HD2	1.77	0.82
1:A:73:GLU:OE2	1:C:2:GLU:HG2	1.79	0.82
2:B:282:THR:HB	2:B:285:THR:HG22	1.61	0.81
1:C:15:TYR:OH	1:C:48:ALA:HB2	1.80	0.81
1:C:212:LEU:HD22	1:C:216:PHE:CZ	2.16	0.81
1:C:48:ALA:O	1:C:52:ILE:HG13	1.81	0.80
2:D:221:VAL:HG22	2:D:281:ILE:HG12	1.64	0.80
1:C:39:THR:O	1:C:40:GLU:HG2	1.83	0.79
1:C:162:GLU:HB3	1:C:164:VAL:HG23	1.62	0.79
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.46	0.79
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.18	0.79
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.63	0.79
2:B:430:LEU:O	2:B:431:ASN:HB2	1.83	0.79
1:A:227:TRP:O	1:A:230:VAL:HG22	1.83	0.77
2:B:282:THR:CB	2:B:285:THR:HG22	2.15	0.76
2:B:207:THR:CG2	2:B:210:MET:HG3	2.13	0.76
2:B:396[B]:GLN:NE2	2:B:400:LYS:NZ	2.37	0.73
2:B:179:HIS:CE1	2:B:320:LEU:HD12	2.24	0.73
1:A:95:ALA:O	1:A:96:LEU:HD23	1.89	0.72
1:A:60:HIS:HD2	1:A:62:ASN:H	1.37	0.72
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.69	0.72
2:B:431:ASN:O	2:B:432:LEU:HB2	1.90	0.72
1:C:64:VAL:HG23	1:C:143:LEU:O	1.91	0.71
2:B:282:THR:O	2:B:285:THR:CG2	2.38	0.71
2:B:309:PRO:HA	2:B:313:GLN:NE2	2.04	0.71
1:A:137:THR:HG22	1:A:296:LEU:CD2	2.21	0.71
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.74	0.70
1:A:39:THR:O	2:B:292:LEU:HD23	1.92	0.69
1:A:245:ARG:NH2	1:A:248:PHE:HE1	1.89	0.69
1:A:38:ASP:N	1:A:38:ASP:OD1	2.25	0.69
1:A:38:ASP:CB	1:A:41:THR:CB	2.63	0.69
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.68
2:D:361:HIS:CE1	2:D:384:LEU:HD21	2.26	0.68
1:A:288:ASP:OD1	1:A:288:ASP:N	2.23	0.67
1:A:71:HIS:CD2	2:B:296:HIS:CD2	2.82	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:HB2	1:A:233:MET:CE	2.24	0.67
2:D:404:HIS:CD2	2:D:406:GLN:H	2.14	0.66
1:A:245:ARG:NH2	1:A:248:PHE:CE1	2.63	0.66
1:A:38:ASP:HB2	1:A:41:THR:CB	2.03	0.66
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.64	0.66
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.78	0.65
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.80	0.65
2:D:207:THR:CG2	2:D:210:MET:HG3	2.23	0.65
1:A:165:THR:CG2	1:A:166:LEU:N	2.59	0.65
1:C:82:PHE:C	1:C:83:LEU:HD12	2.17	0.65
2:D:175:VAL:N	2:D:176:PRO:HD3	2.12	0.65
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.32	0.65
2:D:338:GLU:OE1	2:D:412:LYS:NZ	2.30	0.64
1:C:159:TYR:CE2	2:D:270:ILE:HG23	2.32	0.64
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.32	0.64
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.79	0.64
1:C:162:GLU:HB3	1:C:164:VAL:CG2	2.27	0.64
2:D:278:PHE:O	2:D:281:ILE:HG22	1.97	0.64
1:C:70:ILE:HG22	1:C:70:ILE:O	1.97	0.64
2:D:175:VAL:HG12	2:D:175:VAL:O	1.99	0.63
1:A:41:THR:HG22	1:A:42:GLU:N	2.13	0.63
2:B:275:VAL:HG21	2:B:292:LEU:HD11	1.81	0.63
2:B:404:HIS:O	2:B:407:GLN:NE2	2.31	0.62
1:C:135:ILE:CG2	1:C:141:ILE:HG13	2.22	0.62
2:B:396[B]:GLN:NE2	2:B:400:LYS:HZ2	1.96	0.62
2:B:299:LEU:HD22	2:B:304:PHE:CD1	2.35	0.62
2:D:315:LEU:HD23	2:D:356:ALA:HB1	1.82	0.61
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.83	0.61
2:B:396[B]:GLN:HE22	2:B:400:LYS:NZ	1.97	0.61
2:D:299:LEU:HD22	2:D:304:PHE:CD1	2.35	0.61
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.35	0.61
1:C:173:ILE:HD11	1:C:184:VAL:CG1	2.31	0.61
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.83	0.60
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.82	0.60
1:C:32:LEU:HD23	1:C:79:VAL:HG22	1.82	0.60
1:A:227:TRP:CD2	1:A:230:VAL:CG1	2.83	0.60
2:D:404:HIS:ND1	4:D:2016:HOH:O	2.32	0.60
1:A:163:VAL:O	1:A:163:VAL:CG1	2.44	0.60
2:D:294:MET:O	2:D:298:VAL:HG23	2.02	0.60
1:A:38:ASP:HB3	1:A:41:THR:HB	1.79	0.59
1:A:197:VAL:HG21	1:A:255:LEU:CD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:NH1	1:A:36:ARG:HG3	2.17	0.59
1:A:51:GLU:HG3	1:A:146:PHE:HB2	1.84	0.59
1:C:165:THR:O	1:C:165:THR:HG22	2.03	0.59
2:B:373:PRO:HD2	2:B:376:LEU:HD12	1.85	0.59
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.83	0.59
2:D:207:THR:HG22	2:D:210:MET:CG	2.25	0.58
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.86	0.58
1:A:36:ARG:HG3	1:A:36:ARG:HH11	1.68	0.57
1:A:126:ARG:NH2	1:A:148:LEU:O	2.36	0.57
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.40	0.57
1:A:177:CYS:HB2	1:A:233:MET:HE1	1.85	0.57
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.35	0.57
2:D:335:PHE:CE1	2:D:409:ILE:HG22	2.39	0.57
2:D:361:HIS:C	2:D:361:HIS:CD2	2.77	0.57
1:C:105:LYS:HE2	1:C:285:PHE:O	2.05	0.57
2:B:396[B]:GLN:NE2	2:B:400:LYS:HZ3	2.02	0.56
2:B:309:PRO:HA	2:B:313:GLN:HE22	1.68	0.56
1:A:111:LEU:HD13	1:A:189:LEU:HD11	1.86	0.56
1:C:51:GLU:O	1:C:55:LEU:HB2	2.05	0.56
1:A:237:LYS:NZ	1:A:240:PHE:CE1	2.73	0.56
1:A:13:GLY:C	1:A:15:TYR:N	2.58	0.55
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.41	0.55
1:C:98:GLY:HA2	1:C:199:ARG:HE	1.70	0.55
1:A:71:HIS:CE1	1:A:76:LEU:HD23	2.41	0.55
1:C:251:VAL:HG12	1:C:252:VAL:HG13	1.87	0.55
1:A:122:ARG:HD2	1:A:122:ARG:O	2.07	0.55
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.88	0.55
2:D:240:ASP:O	2:D:244:SER:OG	2.22	0.55
2:D:361:HIS:HE1	2:D:384:LEU:CD2	2.15	0.55
2:B:221:VAL:CG2	2:B:281:ILE:HD12	2.36	0.55
1:A:227:TRP:CE3	1:A:230:VAL:HG11	2.41	0.55
2:D:186:LEU:HD22	2:D:309:PRO:HB3	1.88	0.55
1:C:166:LEU:HD21	1:C:207:SER:C	2.28	0.54
2:B:396[B]:GLN:HE22	2:B:400:LYS:HZ2	1.52	0.54
1:C:15:TYR:HD2	1:C:15:TYR:O	1.91	0.54
1:C:49:ILE:O	1:C:53:SER:OG	2.26	0.54
2:D:207:THR:HG22	2:D:210:MET:H	1.72	0.54
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.90	0.53
1:C:37:LEU:HD12	1:C:39:THR:OG1	2.07	0.53
1:C:37:LEU:HB2	1:C:74:ASN:O	2.08	0.53
1:C:291:LYS:N	1:C:292:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:HD23	1:C:78:LEU:N	2.21	0.53
2:B:275:VAL:HG11	2:B:292:LEU:HD13	1.90	0.53
2:D:176:PRO:HD2	2:D:179:HIS:ND1	2.23	0.53
1:A:248:PHE:HA	1:A:251:VAL:HG23	1.90	0.52
1:C:154:VAL:HG21	2:D:312:ASN:ND2	2.24	0.52
1:A:148:LEU:HD13	1:A:164:VAL:HG13	1.90	0.52
2:B:178:TYR:O	2:B:179:HIS:C	2.48	0.52
1:C:132:ASN:O	1:C:144:ALA:HB3	2.10	0.52
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.97	0.52
2:B:240:ASP:O	2:B:244:SER:HB2	2.09	0.52
1:A:125:HIS:O	1:A:126:ARG:HB2	2.09	0.52
1:A:293:VAL:HG23	1:A:294:PRO:O	2.10	0.52
1:A:231:THR:HA	1:A:236:TYR:CD1	2.45	0.51
1:C:198:THR:O	1:C:199:ARG:HB2	2.09	0.51
1:A:291:LYS:N	1:A:292:PRO:CD	2.73	0.51
1:A:197:VAL:HG21	1:A:255:LEU:HD21	1.90	0.51
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.91	0.51
1:A:52:ILE:CD1	1:A:78:LEU:HD21	2.39	0.51
1:A:71:HIS:CE1	2:B:296:HIS:CD2	2.99	0.51
1:C:60:HIS:HD2	1:C:62:ASN:H	1.58	0.51
1:A:56:LYS:HZ2	1:A:56:LYS:HB3	1.76	0.51
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.93	0.51
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.23	0.51
1:A:165:THR:HG22	1:A:166:LEU:N	2.26	0.51
2:B:227:LEU:HD12	2:B:261:MET:CE	2.42	0.51
1:C:165:THR:HG23	1:C:166:LEU:N	2.26	0.50
1:C:34:LYS:HG3	1:C:77:TYR:CE2	2.46	0.50
2:B:366:THR:HG23	2:B:427:PRO:HD3	1.93	0.50
2:B:263:LEU:HD21	2:B:295:GLU:HG2	1.94	0.50
1:A:121:HIS:O	1:A:123:VAL:HG23	2.11	0.50
1:A:5:GLN:HB2	1:A:24:LYS:HD2	1.93	0.50
1:C:212:LEU:CD2	1:C:216:PHE:CZ	2.91	0.50
2:B:262:LEU:HD13	2:B:278:PHE:CD2	2.46	0.50
2:D:425:ASN:O	2:D:426:PRO:C	2.48	0.50
2:B:236:VAL:HG21	2:B:341:LEU:HD22	1.94	0.49
2:B:299:LEU:HD22	2:B:304:PHE:CE1	2.47	0.49
1:C:91:MET:HE3	1:C:196:MET:CG	2.42	0.49
2:D:376:LEU:O	2:D:380:THR:HG23	2.12	0.49
1:A:60:HIS:CG	1:A:61:PRO:CD	2.95	0.49
1:A:212:LEU:CD2	1:A:216:PHE:CZ	2.92	0.49
2:B:323:GLN:O	2:B:323:GLN:NE2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:OD1	1:A:140:ALA:HB3	2.12	0.49
2:D:418:TYR:O	2:D:421:VAL:HG22	2.12	0.49
1:A:59:ASN:C	1:A:59:ASN:OD1	2.51	0.49
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.13	0.49
2:D:361:HIS:CE1	2:D:384:LEU:CD2	2.93	0.49
2:B:179:HIS:HE1	2:B:320:LEU:HD12	1.74	0.49
2:D:384:LEU:HD12	2:D:384:LEU:O	2.13	0.49
2:B:221:VAL:CG2	2:B:281:ILE:CD1	2.91	0.48
1:C:73:GLU:OE1	2:D:293:ARG:NH2	2.46	0.48
2:B:178:TYR:O	2:B:180:GLU:N	2.47	0.48
1:C:71:HIS:HE1	2:D:304:PHE:HZ	1.62	0.48
2:D:226:LYS:HB2	2:D:226:LYS:NZ	2.28	0.48
2:D:340:SER:OG	2:D:355:ILE:HD13	2.14	0.48
1:A:28:GLU:HG2	1:A:30:VAL:HG13	1.96	0.48
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.96	0.48
1:A:175:LEU:HD23	1:A:212:LEU:HD11	1.95	0.48
2:B:297:LEU:HD12	2:B:297:LEU:O	2.14	0.48
2:B:416:SER:C	2:B:418:TYR:N	2.66	0.48
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.35	0.47
1:A:159:TYR:CD1	2:B:270:ILE:HG23	2.49	0.47
1:C:60:HIS:CG	1:C:61:PRO:CD	2.97	0.47
1:A:115:LEU:HD13	1:A:119:HIS:CE1	2.49	0.47
2:B:323:GLN:HE21	2:B:323:GLN:C	2.18	0.47
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.50	0.47
1:A:170:ALA:HB3	1:A:173:ILE:HG13	1.97	0.47
2:B:221:VAL:HG22	2:B:281:ILE:HD12	1.96	0.47
2:B:416:SER:C	2:B:418:TYR:H	2.18	0.47
2:B:239:ILE:HG22	2:B:243:LEU:HD12	1.96	0.46
1:C:159:TYR:O	1:C:160:THR:C	2.54	0.46
1:C:91:MET:HE3	1:C:196:MET:HG3	1.96	0.46
2:D:412:LYS:HD3	2:D:413:TYR:CE1	2.51	0.46
2:B:221:VAL:HG21	2:B:281:ILE:HD12	1.97	0.46
1:C:159:TYR:O	1:C:162:GLU:HG2	2.15	0.46
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.54	0.46
1:C:291:LYS:N	1:C:292:PRO:HD3	2.31	0.46
2:B:190:GLU:OE1	2:B:352:PRO:HG2	2.16	0.46
1:C:252:VAL:O	1:C:252:VAL:HG23	2.16	0.46
1:A:159:TYR:HB3	1:A:161:HIS:O	2.15	0.45
1:C:51:GLU:HG3	1:C:146:PHE:HB2	1.98	0.45
1:A:115:LEU:HD22	1:A:115:LEU:HA	1.83	0.45
1:C:101:LEU:N	1:C:102:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:335:PHE:HE1	2:D:409:ILE:HG22	1.81	0.45
1:C:39:THR:O	1:C:40:GLU:CG	2.60	0.45
2:B:289:LYS:HE3	2:B:293:ARG:HH12	1.81	0.45
2:D:220:GLU:HG3	2:D:408:SER:OG	2.17	0.45
2:D:388:LYS:HB3	2:D:389:PRO:CD	2.47	0.45
2:D:238:TYR:OH	2:D:306:LEU:HB3	2.17	0.45
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.51	0.45
1:C:188:SER:O	1:C:192:ILE:HG13	2.16	0.45
1:A:55:LEU:HD11	1:A:146:PHE:CE1	2.52	0.45
1:A:71:HIS:HE2	2:B:296:HIS:HD2	1.58	0.45
1:C:220:GLY:O	1:C:269:TYR:OH	2.27	0.45
1:A:275:ILE:HD11	1:A:280:ALA:HA	1.99	0.44
1:C:64:VAL:CG2	1:C:143:LEU:O	2.64	0.44
1:A:111:LEU:CD2	1:A:133:LEU:HD22	2.47	0.44
1:A:170:ALA:HB1	1:A:172:GLU:OE2	2.17	0.44
1:A:210:ASP:O	1:A:214:ARG:HG3	2.17	0.44
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.31	0.44
2:B:360:PHE:HD2	2:B:372:TRP:CZ3	2.34	0.44
1:C:15:TYR:OH	1:C:35:ILE:HD13	2.18	0.44
1:C:28:GLU:HG2	1:C:30:VAL:CG1	2.46	0.44
1:C:158:THR:OG1	1:C:178:LYS:O	2.35	0.44
2:D:402:PRO:HB3	2:D:410:ARG:CZ	2.47	0.44
1:A:174:LEU:HD11	1:A:211:GLN:HG3	2.00	0.44
1:A:248:PHE:HE2	1:A:263:LEU:HG	1.83	0.44
2:B:179:HIS:CD2	2:B:379:LYS:HZ1	2.27	0.44
2:B:338:GLU:HB3	2:B:409:ILE:HD13	1.99	0.44
2:D:373:PRO:O	2:D:377:ILE:HD12	2.17	0.44
1:C:35:ILE:HD13	1:C:35:ILE:HG21	1.61	0.44
1:A:284:PRO:O	1:A:286:PHE:N	2.51	0.44
1:A:293:VAL:O	1:A:293:VAL:CG2	2.61	0.44
2:B:221:VAL:HG21	2:B:281:ILE:CD1	2.48	0.44
1:C:28:GLU:HG2	1:C:30:VAL:HG12	1.99	0.44
1:A:83:LEU:HD11	1:A:142:LYS:HD2	2.00	0.43
1:A:105:LYS:HE2	1:A:285:PHE:O	2.18	0.43
1:A:284:PRO:O	1:A:285:PHE:C	2.55	0.43
2:B:218:LEU:HD22	2:B:261:MET:SD	2.58	0.43
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.53	0.43
2:D:417:LYS:HD2	2:D:418:TYR:CE2	2.53	0.43
2:B:207:THR:HG23	2:B:210:MET:H	1.84	0.43
1:C:15:TYR:OH	1:C:35:ILE:CD1	2.66	0.43
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:C	1:C:78:LEU:HD23	2.39	0.43
1:C:163:VAL:HG13	1:C:163:VAL:O	2.19	0.43
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.00	0.43
1:C:227:TRP:O	1:C:230:VAL:HG12	2.18	0.43
1:A:165:THR:HG23	1:A:166:LEU:N	2.33	0.43
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.99	0.43
1:A:41:THR:HG22	1:A:42:GLU:H	1.82	0.43
1:A:55:LEU:HD11	1:A:146:PHE:CD1	2.54	0.43
2:D:279:VAL:O	2:D:280:TYR:C	2.57	0.43
1:A:159:TYR:CE2	1:A:163:VAL:HG12	2.54	0.43
1:C:221:THR:HA	1:C:222:PRO:HD2	1.76	0.43
2:D:207:THR:CG2	2:D:209:SER:HB3	2.48	0.43
2:D:428:GLU:O	2:D:429:THR:HB	2.19	0.43
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.43
1:C:222:PRO:HB2	1:C:230:VAL:HG21	2.00	0.43
2:B:388:LYS:O	2:B:389:PRO:C	2.57	0.42
1:C:294:PRO:HG2	1:C:296:LEU:HD22	2.01	0.42
2:D:428:GLU:O	2:D:429:THR:CB	2.67	0.42
1:A:255:LEU:HD13	1:A:255:LEU:HA	1.87	0.42
2:B:206:ILE:HD13	2:B:206:ILE:HG21	1.85	0.42
1:C:162:GLU:CB	1:C:164:VAL:HG23	2.41	0.42
2:D:346:PRO:O	2:D:349:LYS:HG3	2.19	0.42
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.79	0.42
2:D:401:ALA:HB1	2:D:410:ARG:HD2	2.01	0.42
1:A:36:ARG:NH1	1:A:36:ARG:CG	2.82	0.42
1:A:49:ILE:HD11	2:B:299:LEU:HD11	2.02	0.42
1:C:60:HIS:CD2	1:C:62:ASN:H	2.37	0.42
1:C:2:GLU:CD	1:C:2:GLU:H	2.21	0.42
1:A:41:THR:CG2	1:A:42:GLU:N	2.79	0.42
1:C:39:THR:CG2	1:C:40:GLU:N	2.82	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.94	0.42
1:C:87:LEU:HD13	1:C:91:MET:SD	2.60	0.42
1:A:33:LYS:HB3	1:A:78:LEU:HB2	2.02	0.41
1:A:175:LEU:HD23	1:A:212:LEU:CD1	2.50	0.41
1:A:247:ASP:O	1:A:250:LYS:N	2.43	0.41
2:B:385:GLU:O	2:B:388:LYS:HB2	2.20	0.41
1:A:207:SER:H	1:A:210:ASP:HB3	1.85	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.83	0.41
1:C:283:HIS:HA	1:C:284:PRO:HD2	1.88	0.41
2:D:297:LEU:O	2:D:301:VAL:HG23	2.19	0.41
1:A:172:GLU:OE2	1:A:172:GLU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:128:LEU:HD11	2.03	0.41
1:A:37:LEU:HB2	1:A:74:ASN:O	2.20	0.41
1:C:161:HIS:O	1:C:162:GLU:C	2.58	0.41
2:B:322:GLN:HG2	2:B:323:GLN:H	1.86	0.41
2:D:282:THR:O	2:D:283:ASP:HB2	2.20	0.41
2:D:331:SER:HB3	2:D:421:VAL:HG21	2.02	0.41
1:A:255:LEU:HD12	1:A:259:GLY:HA3	2.02	0.41
1:C:109:PHE:CE2	1:C:113:GLN:NE2	2.89	0.41
1:A:56:LYS:HZ3	1:A:56:LYS:HG2	1.73	0.41
1:A:99:ILE:HG23	1:A:103:LEU:HD23	2.02	0.41
1:A:121:HIS:O	1:A:122:ARG:C	2.58	0.41
1:C:81:GLU:HG3	1:C:83:LEU:HD11	2.02	0.41
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.56	0.41
1:A:95:ALA:O	1:A:96:LEU:CD2	2.65	0.41
1:A:231:THR:HA	1:A:236:TYR:CE1	2.56	0.41
1:A:83:LEU:HD23	1:A:136:ASN:HB3	2.03	0.40
2:D:302:LEU:C	2:D:303:THR:OG1	2.59	0.40
1:A:49:ILE:HG23	2:B:306:LEU:CD1	2.51	0.40
1:A:159:TYR:CD2	1:A:163:VAL:HG12	2.56	0.40
1:A:262:LEU:O	1:A:263:LEU:C	2.60	0.40
2:B:399:LEU:HA	2:B:399:LEU:HD23	1.85	0.40
1:C:9:LYS:HG3	1:C:19:TYR:CE2	2.56	0.40
1:A:64:VAL:O	1:A:64:VAL:HG13	2.21	0.40
1:A:129:LYS:HE3	1:A:132:ASN:HD21	1.87	0.40
2:B:323:GLN:HE21	2:B:323:GLN:CA	2.34	0.40
2:D:175:VAL:N	2:D:176:PRO:CD	2.82	0.40
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.87	0.40
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.22	0.40
1:A:202:LEU:HD22	1:A:203:PHE:CE1	2.56	0.40
1:C:1:MET:HA	1:C:1:MET:CE	2.51	0.40

There are no symmetry-related clashes.

## 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	A	294/298 (99%)	268 (91%)	22 (8%)	4 (1%)	11	36
1	C	295/298 (99%)	268 (91%)	25 (8%)	2 (1%)	22	54
2	B	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
2	D	256/260 (98%)	240 (94%)	14 (6%)	2 (1%)	19	51
3	E	1/5 (20%)	1 (100%)	0	0	100	100
3	F	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1105/1126 (98%)	1018 (92%)	79 (7%)	8 (1%)	22	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	C	165	THR
2	D	320	LEU
1	A	14	THR
2	D	429	THR
1	A	285	PHE
1	A	164	VAL
1	C	164	VAL

### 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	261/263 (99%)	219 (84%)	42 (16%)	2	7
1	C	261/263 (99%)	231 (88%)	30 (12%)	5	17
2	B	234/234 (100%)	215 (92%)	19 (8%)	11	33
2	D	232/234 (99%)	209 (90%)	23 (10%)	8	24
3	E	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	F	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	992/998 (99%)	876 (88%)	116 (12%)	<b>5</b> <b>16</b>

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	ILE
1	A	12	GLU
1	A	15	TYR
1	A	17	VAL
1	A	22	ARG
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	39	THR
1	A	47	THR
1	A	55	LEU
1	A	56	LYS
1	A	70	ILE
1	A	71	HIS
1	A	73	GLU
1	A	74	ASN
1	A	76	LEU
1	A	89	LYS
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	115	LEU
1	A	122	ARG
1	A	126	ARG
1	A	157	ARG
1	A	160	THR
1	A	164	VAL
1	A	192	ILE
1	A	202	LEU
1	A	212	LEU
1	A	230	VAL
1	A	239	SER
1	A	242	LYS
1	A	246	GLN
1	A	248	PHE
1	A	249	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	251	VAL
1	A	255	LEU
1	A	268	HIS
1	A	287	GLN
1	A	296	LEU
2	B	180	GLU
2	B	200	MET
2	B	201	LYS
2	B	244	SER
2	B	247	SER
2	B	250	ARG
2	B	283	ASP
2	B	288	LYS
2	B	292	LEU
2	B	323	GLN
2	B	343	ASP
2	B	348	LEU
2	B	374	GLU
2	B	391	LEU
2	B	392	MET
2	B	421	VAL
2	B	424	LEU
2	B	430	LEU
2	B	432	LEU
1	C	9	LYS
1	C	14	THR
1	C	15	TYR
1	C	33	LYS
1	C	37	LEU
1	C	42	GLU
1	C	53	SER
1	C	55	LEU
1	C	70	ILE
1	C	71	HIS
1	C	74	ASN
1	C	86	ASP
1	C	87	LEU
1	C	89	LYS
1	C	96	LEU
1	C	115	LEU
1	C	121	HIS
1	C	122	ARG

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Mol	Chain	Res	Type
1	C	131	GLN
1	C	158	THR
1	C	161	HIS
1	C	165	THR
1	C	189	LEU
1	C	200	ARG
1	C	217	ARG
1	C	247	ASP
1	C	268	HIS
1	C	269	TYR
1	C	291	LYS
1	C	296	LEU
2	D	178	TYR
2	D	189	MET
2	D	199	TYR
2	D	207	THR
2	D	226	LYS
2	D	232	LEU
2	D	250	ARG
2	D	283	ASP
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU
2	D	293	ARG
2	D	303	THR
2	D	328	LYS
2	D	340	SER
2	D	364	LEU
2	D	370	GLN
2	D	375	SER
2	D	378	ARG
2	D	384	LEU
2	D	392	MET
2	D	424	LEU
2	D	431	ASN
3	E	2	ARG
3	F	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	246	GLN
1	A	272	ASN
1	A	287	GLN
2	B	208	ASN
2	B	296	HIS
2	B	317	GLN
2	B	323	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	131	GLN
2	D	208	ASN
2	D	229	ASN
2	D	296	HIS
2	D	312	ASN
2	D	322	GLN
2	D	361	HIS
2	D	370	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
3	PFF	E	4	3	11,12,13	0.78	0	12,15,17	2.04	6 (50%)
3	L3O	F	3	3	7,9,10	0.54	0	6,11,13	0.95	0
3	L3O	E	3	3	7,9,10	0.77	0	6,11,13	1.68	2 (33%)
3	PFF	F	4	3	11,12,13	0.52	0	12,15,17	1.54	1 (8%)

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	PFF	E	4	3	-	0/5/6/8	0/1/1/1
3	L3O	F	3	3	-	1/9/10/12	-
3	L3O	E	3	3	-	0/9/10/12	-
3	PFF	F	4	3	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	PFF	CG-CB-CA	-3.94	106.12	114.10
3	E	3	L3O	OZ-CZ-C	-3.24	102.43	110.08
3	E	4	PFF	F-CZ-CE1	3.20	123.97	118.54
3	E	4	PFF	CG-CB-CA	-3.15	107.72	114.10
3	E	4	PFF	CE2-CD2-CG	-2.71	117.30	121.03
3	E	4	PFF	CD2-CE2-CZ	2.50	120.95	118.36
3	E	4	PFF	CD2-CG-CD1	2.46	122.04	118.17
3	E	3	L3O	CD1-CG-CB	2.29	119.52	111.11
3	E	4	PFF	F-CZ-CE2	-2.19	114.83	118.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	L3O	O-C-CZ-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/298 (99%)	0.32	31 (10%) 6 5	29, 51, 78, 89	0
1	C	297/298 (99%)	0.29	33 (11%) 5 4	27, 49, 78, 88	0
2	B	258/260 (99%)	0.20	12 (4%) 31 28	25, 50, 76, 92	0
2	D	258/260 (99%)	0.27	20 (7%) 13 10	25, 50, 77, 89	0
3	E	2/5 (40%)	0.15	0 100 100	55, 55, 55, 89	0
3	F	2/5 (40%)	1.07	0 100 100	75, 75, 75, 87	0
All	All	1113/1126 (98%)	0.27	96 (8%) 10 8	25, 50, 78, 92	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	ARG	7.7
2	B	175	VAL	6.5
1	C	37	LEU	6.3
1	A	230	VAL	5.5
2	D	323	GLN	5.3
1	C	96	LEU	5.3
1	C	17	VAL	5.2
2	D	403	GLN	5.1
1	A	231	THR	5.1
1	C	38	ASP	5.1
1	C	15	TYR	4.8
1	C	39	THR	4.8
1	C	161	HIS	4.6
1	A	95	ALA	4.3
1	A	234	PRO	3.8
1	A	160	THR	3.8
1	A	232	SER	3.7
1	C	40	GLU	3.7
2	B	177	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	228	PRO	3.6
2	D	176	PRO	3.6
2	D	415	ASN	3.6
1	C	14	THR	3.6
1	A	257	GLU	3.6
1	C	232	SER	3.5
1	C	41	THR	3.5
1	A	72	THR	3.4
1	C	231	THR	3.4
1	A	92	ASP	3.3
1	A	233	MET	3.2
2	D	402	PRO	3.2
2	D	175	VAL	3.2
2	B	415	ASN	3.2
1	A	93	ALA	3.1
1	A	249	SER	3.1
1	A	36	ARG	3.0
1	C	163	VAL	3.0
2	D	422	SER	3.0
1	A	178	LYS	3.0
1	A	96	LEU	3.0
1	C	13	GLY	3.0
1	C	16	GLY	2.9
1	C	206	ASP	2.9
1	C	36	ARG	2.9
1	C	199	ARG	2.9
1	C	97	THR	2.8
1	A	37	LEU	2.8
1	C	74	ASN	2.8
2	B	416	SER	2.8
1	C	162	GLU	2.8
2	D	324	PRO	2.8
2	B	419	HIS	2.8
1	A	74	ASN	2.8
1	A	40	GLU	2.7
1	C	229	GLY	2.7
1	A	161	HIS	2.7
2	B	418	TYR	2.7
1	C	296	LEU	2.7
1	A	229	GLY	2.7
1	A	205	GLY	2.6
1	A	94	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	2.6
1	C	12	GLU	2.6
2	B	378	ARG	2.6
2	D	325	ALA	2.6
1	A	71	HIS	2.6
1	A	39	THR	2.6
1	A	177	CYS	2.6
2	B	377	ILE	2.6
1	A	176	GLY	2.5
2	D	284	ASP	2.5
2	D	401	ALA	2.5
1	C	224	GLU	2.5
1	C	98	GLY	2.5
2	B	176	PRO	2.5
1	C	11	GLY	2.5
2	D	414	LYS	2.5
2	D	239	ILE	2.5
2	B	201	LYS	2.4
2	D	192	LYS	2.4
2	B	236	VAL	2.4
2	D	177	ASP	2.4
2	D	178	TYR	2.4
1	C	226	VAL	2.4
2	D	280	TYR	2.3
1	C	73	GLU	2.3
1	A	227	TRP	2.2
1	A	38	ASP	2.2
2	D	257	GLY	2.2
2	D	416	SER	2.1
2	D	341	LEU	2.1
1	C	19	TYR	2.1
1	A	162	GLU	2.1
1	C	225	VAL	2.1
1	A	236	TYR	2.0
2	B	324	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PFF	E	4	12/13	0.92	0.17	54,57,63,64	0
3	L3O	E	3	10/11	0.95	0.20	31,55,59,66	0
3	PFF	F	4	12/13	0.95	0.35	60,63,80,89	0
3	L3O	F	3	10/11	0.96	0.29	46,53,60,61	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.