



# Full wwPDB X-ray Structure Validation Report i

May 15, 2020 – 05:39 pm BST

PDB ID : 5U7Q

Title : Identification of A New Class of Potent Cdc7 Inhibitors Designed by Putative Pharmacophore Model: Synthesis and Biological Evaluation of 2,3-Dihydrothieno[3,2-d]pyrimidin-4(1H)-ones

Authors : Hoffman, I.D.

Deposited on : 2016-12-12

Resolution : 3.15 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 i symbol.

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The following versions of software and data (see references ①) were used in the production of this report:

MolProbity : 4.02b-467

Xtriage (Phenix) : 1.13

EDS : 2.11

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) : 2.11

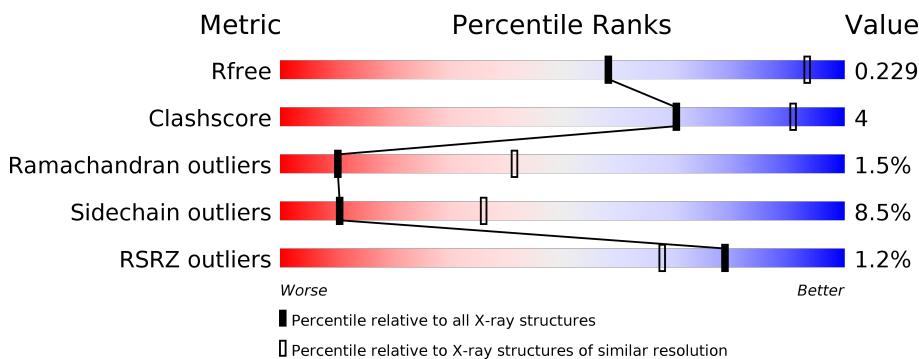
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

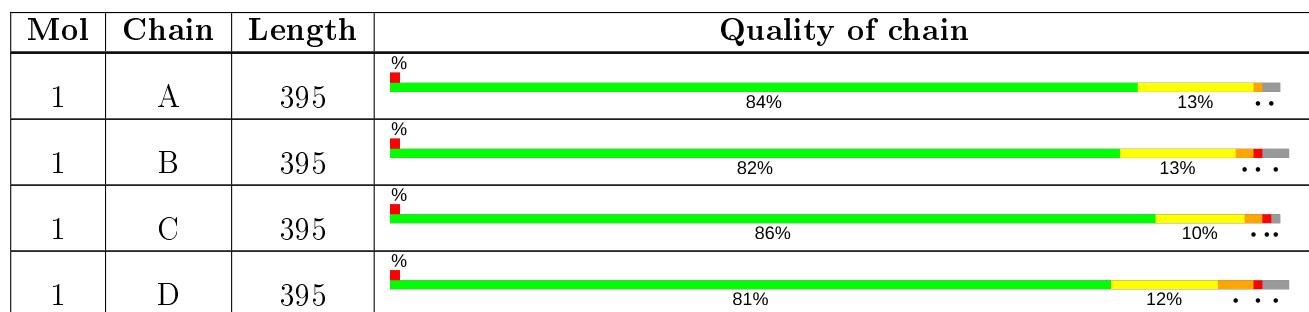
The reported resolution of this entry is 3.15 Å.

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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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 <=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.



## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12540 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 Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3147	2018	528	581	20			
1	B	385	Total	C	N	O	S	0	0	0
			3121	2004	521	576	20			
1	C	390	Total	C	N	O	S	0	0	0
			3156	2023	530	583	20			
1	D	383	Total	C	N	O	S	0	0	0
			3106	1996	518	573	19			

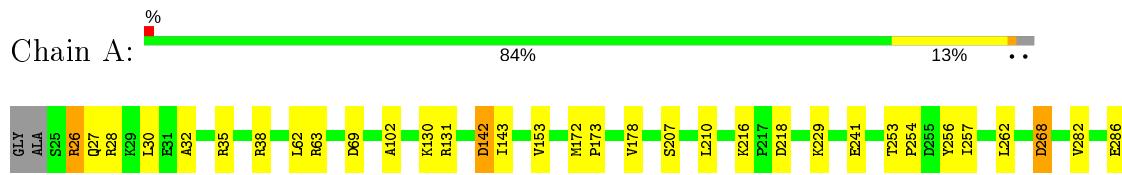
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	3	Total O 3 3	0	0
2	C	2	Total O 2 2	0	0
2	D	3	Total O 3 3	0	0

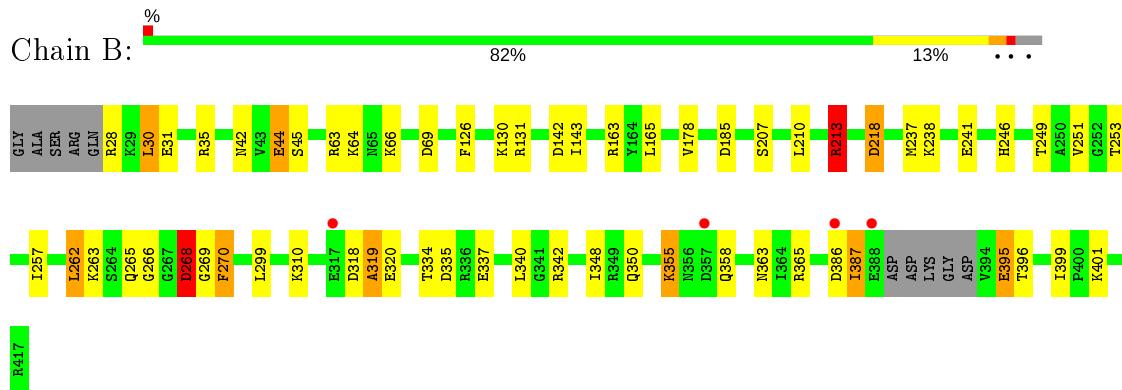
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

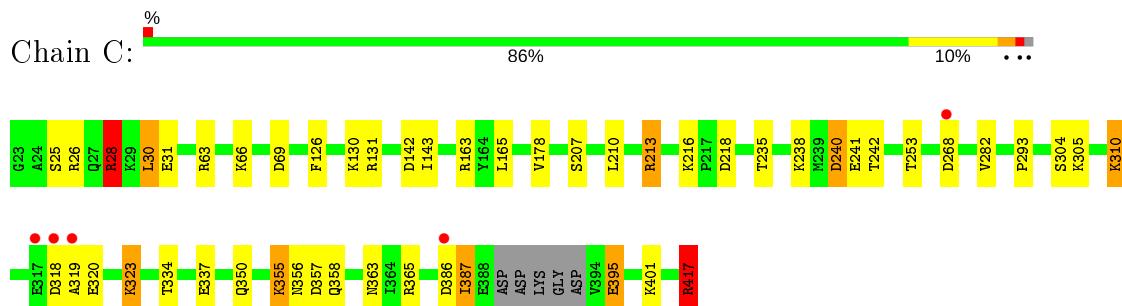
- Molecule 1: Rho-associated protein kinase 2



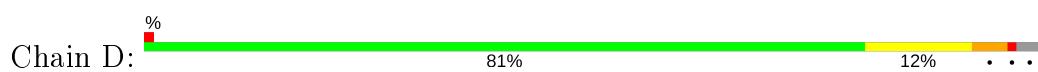
- Molecule 1: Rho-associated protein kinase 2

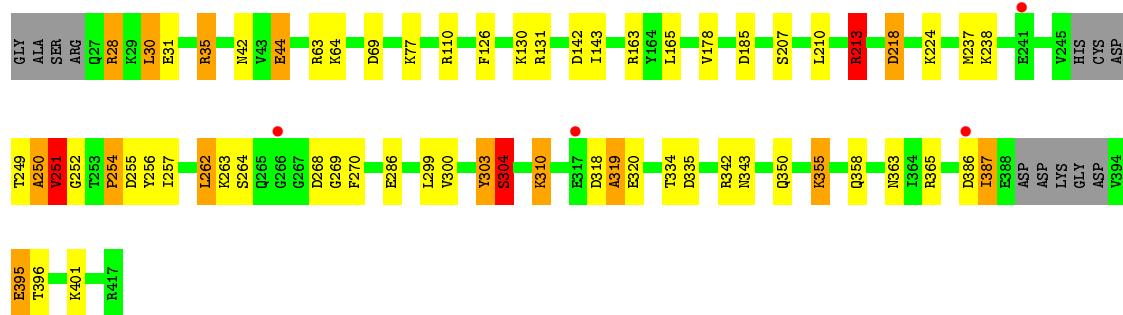


- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.19 Å    146.46 Å    112.42 Å 90.00°    96.34°    90.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.83 – 3.12	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-3.15) 98.1 (29.83-3.12)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.68 (at 3.11 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
$R$ , $R_{free}$	0.205 , 0.235 0.203 , 0.229	Depositor DCC
$R_{free}$ test set	2611 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.4	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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  $< |L| >$ ,  $< L^2 >$  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

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	0.58	0/3225	0.85	8/4357 (0.2%)
1	B	0.55	0/3199	0.86	4/4323 (0.1%)
1	C	0.55	0/3234	0.84	5/4369 (0.1%)
1	D	0.57	0/3182	0.88	8/4298 (0.2%)
All	All	0.56	0/12840	0.86	25/17347 (0.1%)

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	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	270	PHE	CB-CG-CD1	9.17	127.22	120.80
1	D	213	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	B	213	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	D	304	SER	N-CA-CB	8.71	123.57	110.50
1	B	270	PHE	CB-CG-CD2	-8.61	114.78	120.80
1	C	357	ASP	CB-CG-OD2	7.42	124.98	118.30
1	D	355	LYS	CA-CB-CG	7.25	129.35	113.40
1	C	417	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	D	303	TYR	N-CA-C	-7.04	91.99	111.00
1	A	142	ASP	CB-CG-OD1	6.32	123.99	118.30
1	C	28	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	268	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	PHE	N-CA-CB	6.27	121.89	110.60
1	D	35	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	240	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	403	PHE	N-CA-C	-5.90	95.06	111.00
1	C	357	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	D	110	ARG	CG-CD-NE	5.79	123.95	111.80
1	A	355	LYS	CD-CE-NZ	5.49	124.32	111.70
1	A	336	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	335	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	213	ARG	CD-NE-CZ	5.24	130.94	123.60
1	B	268	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	30	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	26	ARG	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	246	HIS	Peptide
1	B	269	GLY	Peptide
1	D	251	VAL	Peptide
1	D	252	GLY	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	3147	0	3074	31	0
1	B	3121	0	3048	17	0
1	C	3156	0	3082	19	0
1	D	3106	0	3039	25	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	1	0
All	All	12540	0	12243	88	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 4.

All (88) 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:172:MET:CE	1:A:229:LYS:HD2	1.72	1.19
1:A:172:MET:HE1	1:A:229:LYS:CD	1.82	1.08
1:A:153:VAL:HG22	1:A:172:MET:CE	2.09	0.83
1:A:153:VAL:HG22	1:A:172:MET:HE3	1.62	0.82
1:A:172:MET:HE1	1:A:229:LYS:HD2	0.89	0.81
1:D:28:ARG:H	1:D:28:ARG:HD2	1.55	0.71
1:D:257:ILE:HG21	1:D:262:LEU:HD13	1.72	0.70
1:A:62:LEU:HD21	1:A:402:ALA:O	1.94	0.68
1:B:257:ILE:HG21	1:B:262:LEU:HD13	1.76	0.67
1:D:264:SER:HB2	1:D:269:GLY:HA3	1.78	0.66
1:D:213:ARG:HH11	1:D:213:ARG:HG2	1.60	0.65
1:A:394:VAL:O	1:A:395:GLU:OE1	2.15	0.65
1:D:300:VAL:O	1:D:303:TYR:O	2.14	0.64
1:C:323:LYS:HG3	1:D:343:ASN:HD21	1.62	0.64
1:A:216:LYS:NZ	1:A:253:THR:HG21	2.12	0.64
1:C:216:LYS:NZ	1:C:253:THR:HG21	2.12	0.63
1:D:254:PRO:O	1:D:256:TYR:N	2.32	0.62
1:C:355:LYS:HE3	1:C:356:ASN:H	1.66	0.61
1:C:240:ASP:OD1	1:C:242:THR:OG1	2.18	0.60
1:A:102:ALA:HB1	1:A:131:ARG:HH12	1.67	0.59
1:A:173:PRO:HB2	1:A:375:LEU:HD21	1.82	0.59
1:C:213:ARG:NH1	1:C:235:THR:O	2.35	0.59
1:B:268:ASP:OD1	1:B:268:ASP:N	2.37	0.58
1:A:254:PRO:O	1:A:257:ILE:HG22	2.06	0.56
1:A:256:TYR:OH	1:A:286:GLU:OE1	2.18	0.56
1:A:62:LEU:CD2	1:A:402:ALA:O	2.54	0.56
1:B:386:ASP:C	1:B:387:ILE:HG12	2.27	0.55
1:A:262:LEU:HD23	1:A:307:MET:HE3	1.87	0.55
1:C:386:ASP:C	1:C:387:ILE:HG12	2.27	0.55
1:D:386:ASP:C	1:D:387:ILE:HG12	2.27	0.54
1:A:153:VAL:HG22	1:A:172:MET:HE2	1.86	0.54
1:C:323:LYS:HE2	1:C:323:LYS:H	1.72	0.53
1:B:143:ILE:HD11	1:B:210:LEU:HD13	1.90	0.52
1:A:143:ILE:HD11	1:A:210:LEU:HD13	1.92	0.52
1:D:143:ILE:HD11	1:D:210:LEU:HD13	1.92	0.51
1:B:257:ILE:CG2	1:B:262:LEU:HD13	2.40	0.51
1:C:143:ILE:HD11	1:C:210:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:C	1:A:28:ARG:H	2.15	0.50
1:B:249:THR:O	1:B:265:GLN:NE2	2.44	0.50
1:C:355:LYS:HE3	1:C:356:ASN:N	2.26	0.50
1:A:62:LEU:HD21	1:A:402:ALA:C	2.32	0.50
1:C:25:SER:OG	1:C:28:ARG:HD3	2.11	0.50
1:C:216:LYS:HZ2	1:C:253:THR:HG21	1.77	0.49
1:A:102:ALA:HB1	1:A:131:ARG:NH1	2.27	0.49
1:D:257:ILE:CG2	1:D:262:LEU:HD13	2.40	0.49
1:A:216:LYS:HZ2	1:A:253:THR:HG21	1.78	0.48
1:D:42:ASN:OD1	1:D:44:GLU:HG2	2.14	0.47
1:A:262:LEU:HB3	1:A:307:MET:HE1	1.96	0.47
1:A:38:ARG:NH1	1:A:142:ASP:OD1	2.42	0.47
1:A:63:ARG:NH1	1:A:69:ASP:OD1	2.47	0.46
1:D:63:ARG:NH1	1:D:69:ASP:OD1	2.47	0.46
1:D:28:ARG:HD2	1:D:28:ARG:N	2.27	0.46
1:C:63:ARG:NH1	1:C:69:ASP:OD1	2.48	0.46
1:C:417:ARG:HG3	1:C:417:ARG:HH11	1.81	0.45
1:A:26:ARG:HG3	1:A:28:ARG:NH1	2.31	0.45
1:B:266:GLY:O	1:C:305:LYS:HE2	2.17	0.45
1:B:42:ASN:OD1	1:B:44:GLU:HG2	2.16	0.45
1:C:323:LYS:HG3	1:D:343:ASN:ND2	2.29	0.45
1:D:303:TYR:O	1:D:304:SER:CB	2.65	0.45
1:D:318:ASP:O	1:D:319:ALA:C	2.55	0.44
1:D:256:TYR:OH	1:D:286:GLU:OE1	2.22	0.44
1:D:264:SER:CB	1:D:269:GLY:HA3	2.46	0.44
1:C:310:LYS:HB3	1:D:310:LYS:HD3	1.98	0.43
1:B:63:ARG:NH1	1:B:69:ASP:OD1	2.47	0.43
1:D:251:VAL:HG12	2:D:503:HOH:O	2.18	0.43
1:A:374:GLU:C	1:A:375:LEU:HD12	2.39	0.43
1:B:318:ASP:O	1:B:319:ALA:C	2.55	0.43
1:B:318:ASP:O	1:B:320:GLU:HG3	2.19	0.43
1:C:126:PHE:CD1	1:C:395:GLU:HG2	2.54	0.43
1:D:250:ALA:O	1:D:251:VAL:HB	2.19	0.43
1:A:373:PRO:HB2	1:A:375:LEU:CD1	2.49	0.42
1:D:318:ASP:O	1:D:320:GLU:HG3	2.19	0.42
1:B:251:VAL:HG13	1:B:265:GLN:OE1	2.19	0.42
1:A:32:ALA:O	1:A:35:ARG:HG2	2.20	0.42
1:B:355:LYS:HA	1:B:355:LYS:HE3	2.02	0.42
1:D:126:PHE:CD1	1:D:395:GLU:HG2	2.55	0.42
1:B:340:LEU:HG	1:B:348:ILE:HG12	2.02	0.42
1:D:264:SER:HB2	1:D:269:GLY:CA	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASP:OD1	1:B:218:ASP:N	2.52	0.41
1:A:282:VAL:HG13	1:A:293:PRO:HD2	2.03	0.41
1:A:318:ASP:O	1:A:320:GLU:HG3	2.21	0.41
1:B:126:PHE:CD1	1:B:395:GLU:HG2	2.56	0.41
1:A:386:ASP:C	1:A:387:ILE:HG13	2.42	0.41
1:B:213:ARG:O	1:B:213:ARG:HD2	2.21	0.41
1:A:408:LEU:N	1:A:409:PRO:CD	2.84	0.41
1:C:318:ASP:O	1:C:320:GLU:HG3	2.21	0.41
1:C:282:VAL:HG13	1:C:293:PRO:HD2	2.03	0.40
1:D:218:ASP:N	1:D:218:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	384/395 (97%)	368 (96%)	11 (3%)	5 (1%)	12 44
1	B	381/395 (96%)	364 (96%)	13 (3%)	4 (1%)	15 51
1	C	386/395 (98%)	371 (96%)	10 (3%)	5 (1%)	12 44
1	D	377/395 (95%)	359 (95%)	9 (2%)	9 (2%)	6 30
All	All	1528/1580 (97%)	1462 (96%)	43 (3%)	23 (2%)	10 41

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	ASP
1	B	395	GLU
1	C	268	ASP
1	C	395	GLU
1	D	250	ALA

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Mol	Chain	Res	Type
1	D	251	VAL
1	D	255	ASP
1	D	304	SER
1	D	395	GLU
1	A	395	GLU
1	A	403	PHE
1	B	253	THR
1	C	28	ARG
1	D	254	PRO
1	D	268	ASP
1	B	319	ALA
1	D	319	ALA
1	A	319	ALA
1	B	30	LEU
1	C	319	ALA
1	D	30	LEU
1	A	27	GLN
1	C	30	LEU

### 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	342/346 (99%)	331 (97%)	11 (3%)	39 70
1	B	339/346 (98%)	299 (88%)	40 (12%)	5 21
1	C	342/346 (99%)	313 (92%)	29 (8%)	10 36
1	D	337/346 (97%)	301 (89%)	36 (11%)	6 25
All	All	1360/1384 (98%)	1244 (92%)	116 (8%)	10 36

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

Mol	Chain	Res	Type
1	A	130	LYS
1	A	178	VAL
1	A	207	SER

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Mol	Chain	Res	Type
1	A	218	ASP
1	A	241	GLU
1	A	304	SER
1	A	334	THR
1	A	358	GLN
1	A	365	ARG
1	A	395	GLU
1	A	396	THR
1	B	28	ARG
1	B	30	LEU
1	B	31	GLU
1	B	35	ARG
1	B	44	GLU
1	B	45	SER
1	B	64	LYS
1	B	66	LYS
1	B	130	LYS
1	B	131	ARG
1	B	142	ASP
1	B	163	ARG
1	B	165	LEU
1	B	178	VAL
1	B	185	ASP
1	B	207	SER
1	B	213	ARG
1	B	218	ASP
1	B	237	MET
1	B	238	LYS
1	B	241	GLU
1	B	262	LEU
1	B	263	LYS
1	B	268	ASP
1	B	270	PHE
1	B	299	LEU
1	B	310	LYS
1	B	334	THR
1	B	335	ASP
1	B	337	GLU
1	B	342	ARG
1	B	350	GLN
1	B	355	LYS
1	B	358	GLN

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Mol	Chain	Res	Type
1	B	363	ASN
1	B	365	ARG
1	B	387	ILE
1	B	396	THR
1	B	399	ILE
1	B	401	LYS
1	C	26	ARG
1	C	28	ARG
1	C	30	LEU
1	C	31	GLU
1	C	66	LYS
1	C	130	LYS
1	C	131	ARG
1	C	142	ASP
1	C	163	ARG
1	C	165	LEU
1	C	178	VAL
1	C	207	SER
1	C	213	ARG
1	C	218	ASP
1	C	238	LYS
1	C	241	GLU
1	C	304	SER
1	C	310	LYS
1	C	323	LYS
1	C	334	THR
1	C	337	GLU
1	C	350	GLN
1	C	355	LYS
1	C	358	GLN
1	C	363	ASN
1	C	365	ARG
1	C	387	ILE
1	C	401	LYS
1	C	417	ARG
1	D	28	ARG
1	D	30	LEU
1	D	31	GLU
1	D	35	ARG
1	D	44	GLU
1	D	64	LYS
1	D	77	LYS

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Mol	Chain	Res	Type
1	D	130	LYS
1	D	131	ARG
1	D	142	ASP
1	D	163	ARG
1	D	165	LEU
1	D	178	VAL
1	D	185	ASP
1	D	207	SER
1	D	213	ARG
1	D	218	ASP
1	D	224	LYS
1	D	237	MET
1	D	238	LYS
1	D	249	THR
1	D	262	LEU
1	D	263	LYS
1	D	270	PHE
1	D	299	LEU
1	D	310	LYS
1	D	334	THR
1	D	342	ARG
1	D	350	GLN
1	D	355	LYS
1	D	358	GLN
1	D	363	ASN
1	D	365	ARG
1	D	387	ILE
1	D	396	THR
1	D	401	LYS

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

Mol	Chain	Res	Type
1	A	107	GLN
1	B	86	GLN
1	B	107	GLN
1	B	363	ASN
1	C	107	GLN
1	C	358	GLN
1	C	363	ASN
1	D	107	GLN
1	D	363	ASN

**5.3.3 RNA** [\(i\)](#)

There are no RNA molecules in this entry.

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

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

**5.5 Carbohydrates** [\(i\)](#)

There are no carbohydrates in this entry.

**5.6 Ligand geometry** [\(i\)](#)

There are no ligands in this entry.

**5.7 Other polymers** [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	388/395 (98%)	-0.29	5 (1%) 77 66	38, 66, 100, 141	0
1	B	385/395 (97%)	-0.26	4 (1%) 82 73	41, 69, 108, 141	0
1	C	390/395 (98%)	-0.27	5 (1%) 77 66	42, 71, 107, 136	0
1	D	383/395 (96%)	-0.23	4 (1%) 82 73	46, 72, 110, 138	0
All	All	1546/1580 (97%)	-0.26	18 (1%) 79 68	38, 70, 108, 141	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	ASP	2.9
1	C	317	GLU	2.8
1	A	317	GLU	2.6
1	B	388	GLU	2.5
1	B	317	GLU	2.4
1	A	388	GLU	2.4
1	A	318	ASP	2.3
1	A	316	PRO	2.3
1	B	386	ASP	2.3
1	D	317	GLU	2.3
1	D	241	GLU	2.2
1	C	268	ASP	2.2
1	D	266	GLY	2.2
1	C	318	ASP	2.2
1	C	386	ASP	2.2
1	D	386	ASP	2.2
1	C	319	ALA	2.1
1	B	357	ASP	2.1

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates 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.