wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:52 AM GMT

PDB ID	:	3NDM
Title	:	Crystal structure of Rho-Associated Protein Kinase (ROCK1) with a potent isoquinolone derivative
Authors	:	Li, X.
Deposited on	:	2010-06-07
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

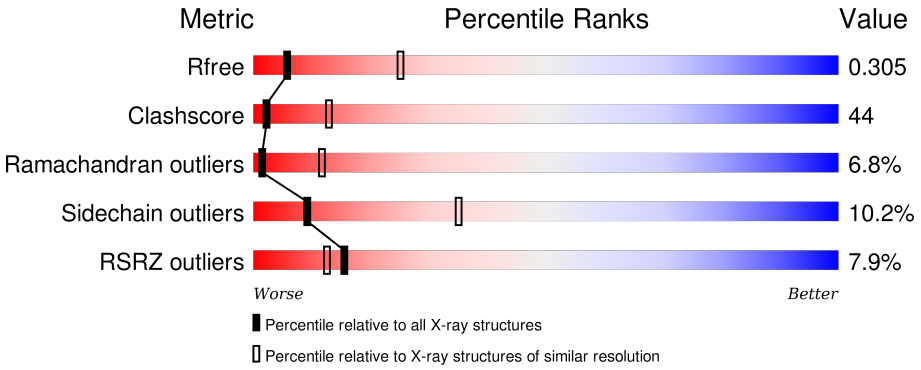
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	A	415	15% 32% 50% 9% • 8%
1	B	415	3% 32% 52% 11% • 5%
1	C	415	9% 31% 48% 9% • 11%
1	D	415	2% 33% 54% 8% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12746 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.

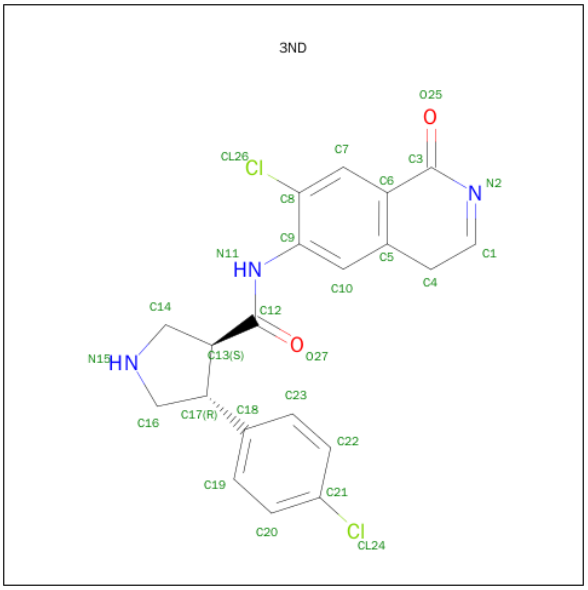
- Molecule 1 is a protein called Rho-Associated Protein Kinase (ROCK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3128	2005	517	584	22			
1	B	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			
1	C	371	Total	C	N	O	S	0	0	0
			3028	1944	493	569	22			
1	D	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q13464
A	2	SER	-	EXPRESSION TAG	UNP Q13464
A	3	LEU	-	EXPRESSION TAG	UNP Q13464
A	4	HIS	-	EXPRESSION TAG	UNP Q13464
A	5	MET	-	EXPRESSION TAG	UNP Q13464
B	1	GLY	-	EXPRESSION TAG	UNP Q13464
B	2	SER	-	EXPRESSION TAG	UNP Q13464
B	3	LEU	-	EXPRESSION TAG	UNP Q13464
B	4	HIS	-	EXPRESSION TAG	UNP Q13464
B	5	MET	-	EXPRESSION TAG	UNP Q13464
C	1	GLY	-	EXPRESSION TAG	UNP Q13464
C	2	SER	-	EXPRESSION TAG	UNP Q13464
C	3	LEU	-	EXPRESSION TAG	UNP Q13464
C	4	HIS	-	EXPRESSION TAG	UNP Q13464
C	5	MET	-	EXPRESSION TAG	UNP Q13464
D	1	GLY	-	EXPRESSION TAG	UNP Q13464
D	2	SER	-	EXPRESSION TAG	UNP Q13464
D	3	LEU	-	EXPRESSION TAG	UNP Q13464
D	4	HIS	-	EXPRESSION TAG	UNP Q13464
D	5	MET	-	EXPRESSION TAG	UNP Q13464

- Molecule 2 is (3S,4R)-N-(7-CHLORO-1-OXO-1,4-DIHYDROISOQUINOLIN-6-YL)-4-(4-C HLOROPHENYL)PYRROLIDINE-3-CARBOXAMIDE (three-letter code: 3ND) (formula: $C_{20}H_{17}Cl_2N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		

- Molecule 3 is water.

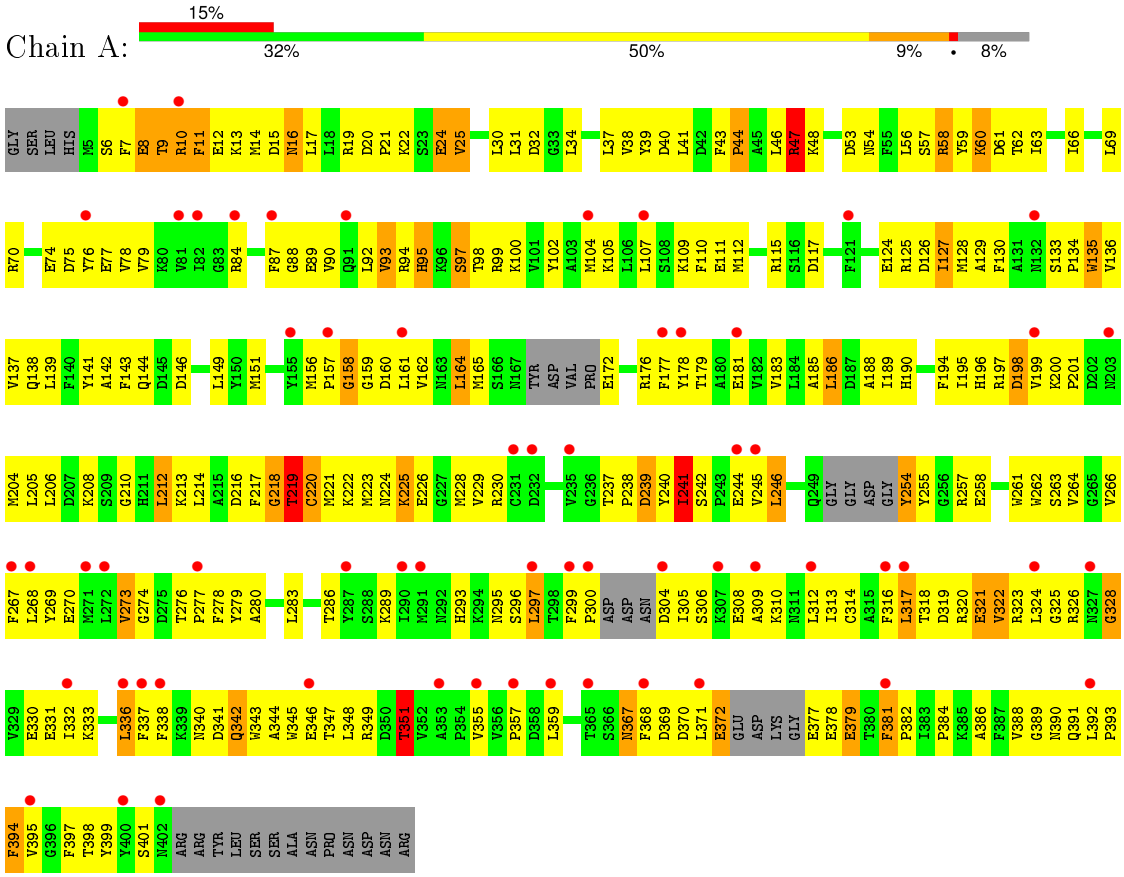
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		
3	C	15	Total	O	0	0
			15	15		
3	D	14	Total	O	0	0
			14	14		

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.

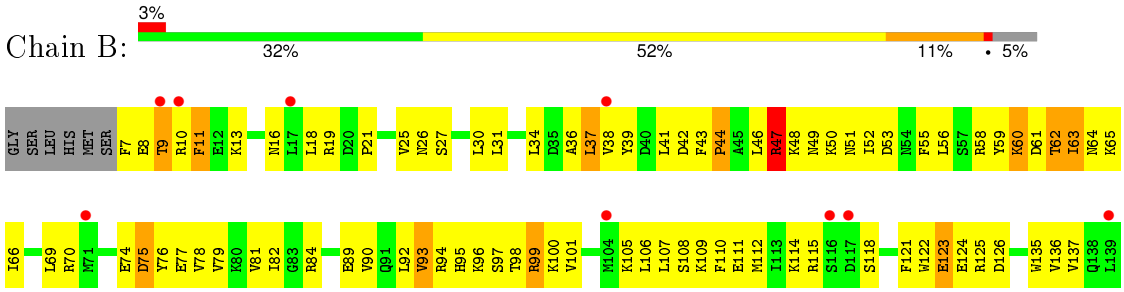
- Molecule 1: Rho-Associated Protein Kinase (ROCK1)

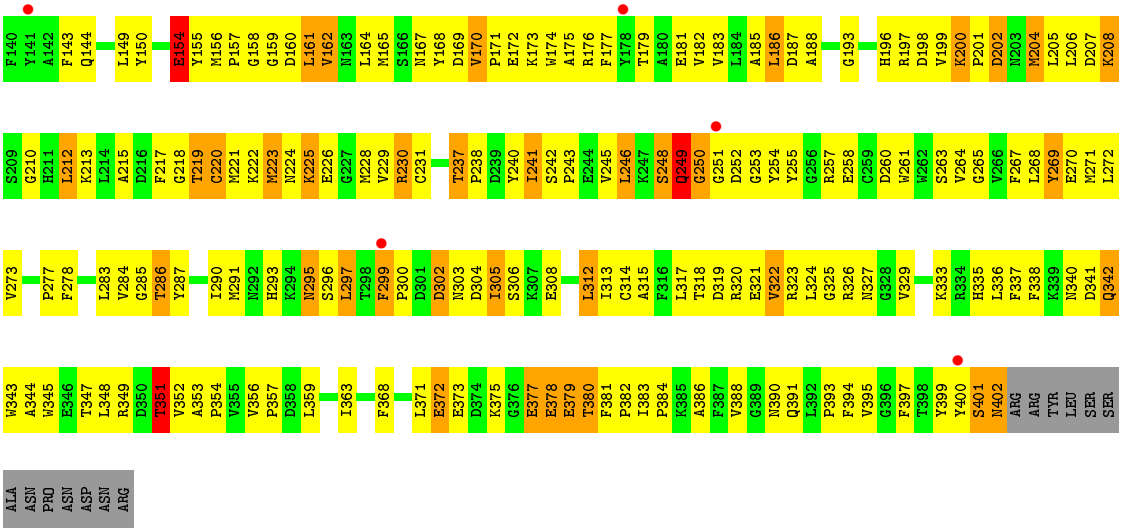
Chain A:



- Molecule 1: Rho-Associated Protein Kinase (ROCK1)

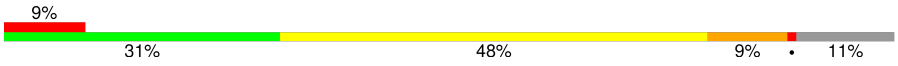
Chain B:

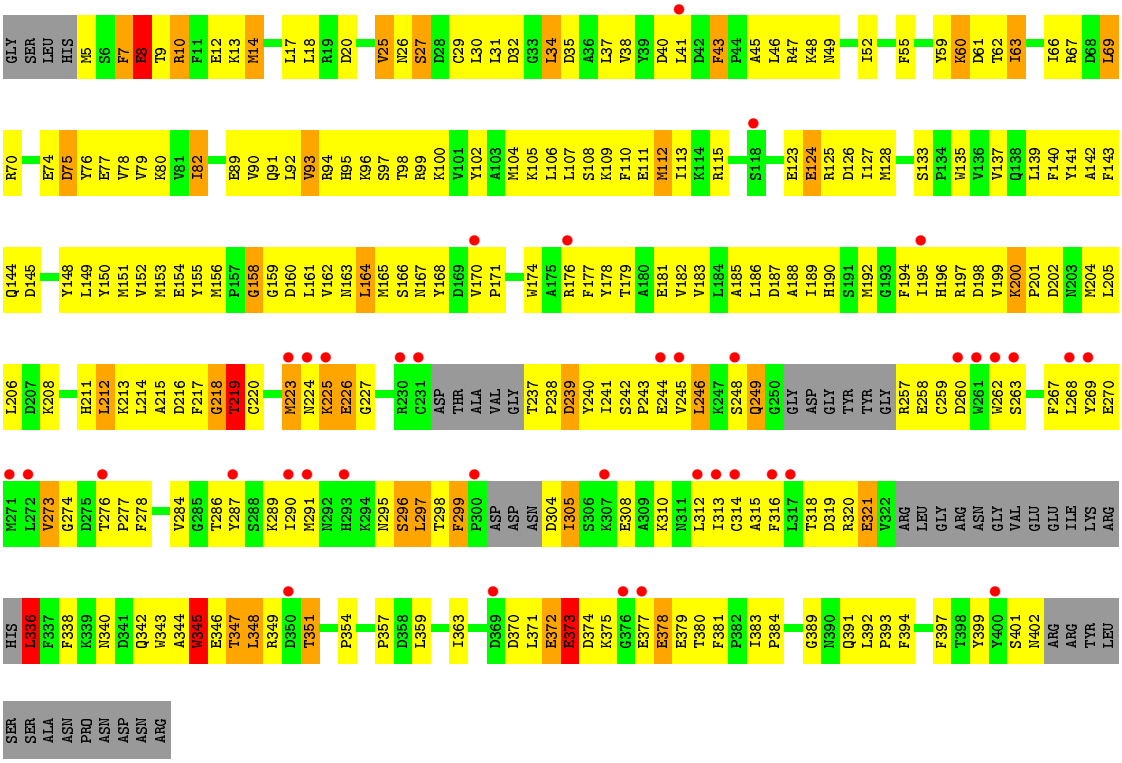




- Molecule 1: Rho-Associated Protein Kinase (ROCK1)

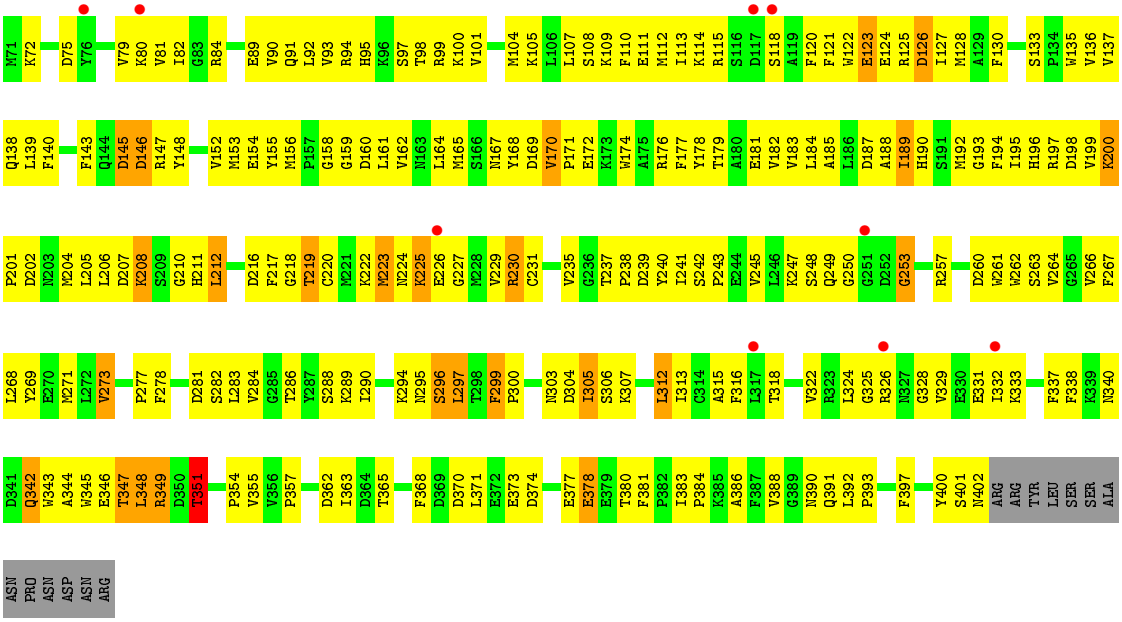
Chain C:





- Molecule 1: Rho-Associated Protein Kinase (ROCK1)

Chain D:


W71 K72 D75 V76 V79 K80 V81 I82 G83 R84 E89 V90 Q91 L92 V93 R94 H95 K96 S97 T98 R99 K100 V101 M104 K105 L106 L107 S108 K109 F110 E111 M112 I113 K114 R115 S116 D117 S118 A119 F120 F121 W122 E123 E124 R125 D126 I127 M128 A129 F130 S133 P134 W135 V136 V137
Q138 L139 F140 F143 Q144 D145 D146 R147 Y148 V152 M153 E154 Y155 M156 P157 G158 G159 D160 L161 V162 N163 L164 M165 S166 N167 Y168 D169 V170 P171 E172 K173 W174 A175 R176 F177 Y178 T179 A180 E181 V182 V183 L184 A185 L186 D187 A188 I189 H190 S191 M192 G193 F194 I195 H196 R197 D198 V199 K200
P201 D202 N203 M204 L205 L206 D207 K208 S209 G210 H211 L212 D216 F217 G218 T219 C220 M221 K222 M223 N224 K225 E226 G227 M228 V229 R230 C231 V235 G236 T237 P238 D239 Y240 I241 S242 P243 E244 V245 L246 K247 S248 Q249 G250 G251 D252 G253 R257 D260 W261 W262 S263 V264 G265 V266 F267
L268 Y269 E270 M271 L272 V273 P277 F278 D281 S282 I283 V284 G285 T286 Y287 S288 R289 I290 K294 N295 S296 I297 T298 F299 P300 N303 D304 I305 S306 K307 I312 I313 C314 A315 F316 L317 T318 V322 R323 I324 G325 R326 N327 G328 V329 E330 E331 I332 K333 F337 F338 K339 N340
D341 Q342 W343 A344 W345 E346 T347 L348 R349 D350 T351 P354 V355 V356 P357 D362 I363 D364 T365 F368 D369 D370 L371 E372 E373 D374 E377 E378 E379 T380 F381 P382 I383 P384 K385 A386 F387 V388 G389 N390 Q391 L392 P393 F397 Y400 S401 N402 ARG ARG TYR LEU SER SER ALA
ASN PRO ASN ASP ASN ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.78Å 83.55Å 177.96Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	42.53 – 3.30 44.72 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.53-3.30) 99.6 (44.72-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.241 , 0.310 0.238 , 0.305	Depositor DCC
R_{free} test set	1402 reflections (4.68%)	DCC
Wilson B-factor (Å^2)	129.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 160.5	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 31334 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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: 3ND

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	0.39	0/3199	0.57	0/4314
1	B	0.55	0/3299	0.67	0/4457
1	C	0.49	0/3098	0.62	1/4180 (0.0%)
1	D	0.56	0/3299	0.67	0/4457
All	All	0.50	0/12895	0.63	1/17408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	336	LEU	CA-CB-CG	-5.52	102.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3128	0	3048	269	0
1	B	3222	0	3120	282	0
1	C	3028	0	2943	304	0
1	D	3222	0	3120	292	0
2	B	27	0	17	7	0
2	C	27	0	17	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	17	5	0
3	A	20	0	0	5	0
3	B	16	0	0	3	0
3	C	15	0	0	5	0
3	D	14	0	0	1	0
All	All	12746	0	12282	1105	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 44.

The worst 5 of 1105 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:66:ILE:HD11	1:B:25:VAL:HG21	1.35	1.08
1:A:399:TYR:CE2	1:A:401:SER:HB2	1.91	1.04
1:A:230:ARG:HH21	1:A:254:TYR:HB2	1.23	1.02
1:C:78:VAL:HA	1:C:93:VAL:HG12	1.42	1.00
1:B:38:VAL:HG21	1:B:63:ILE:HG13	1.41	0.99

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	373/415 (90%)	282 (76%)	65 (17%)	26 (7%)	1 11
1	B	394/415 (95%)	294 (75%)	70 (18%)	30 (8%)	1 9
1	C	361/415 (87%)	268 (74%)	67 (19%)	26 (7%)	1 11
1	D	394/415 (95%)	286 (73%)	86 (22%)	22 (6%)	2 16
All	All	1522/1660 (92%)	1130 (74%)	288 (19%)	104 (7%)	1 12

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	99	ARG
1	A	273	VAL
1	A	351	THR
1	B	60	LYS

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	343/369 (93%)	307 (90%)	36 (10%)	8	33
1	B	352/369 (95%)	312 (89%)	40 (11%)	7	29
1	C	334/369 (90%)	302 (90%)	32 (10%)	10	38
1	D	352/369 (95%)	319 (91%)	33 (9%)	11	39
All	All	1381/1476 (94%)	1240 (90%)	141 (10%)	9	35

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	ILE
1	C	14	MET
1	D	288	SER
1	B	319	ASP
1	B	372	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	ASN
1	C	211	HIS
1	D	327	ASN
1	C	190	HIS
1	C	292	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands 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	$\#\|Z\| > 2$
2	3ND	B	900	-	24,30,30	1.90	3 (12%)	34,43,43	1.99	8 (23%)
2	3ND	C	900	-	24,30,30	1.74	2 (8%)	34,43,43	1.93	8 (23%)
2	3ND	D	900	-	24,30,30	1.86	2 (8%)	34,43,43	1.99	8 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3ND	B	900	-	-	0/12/32/32	0/3/4/4
2	3ND	C	900	-	-	0/12/32/32	0/3/4/4
2	3ND	D	900	-	-	0/12/32/32	0/3/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	3ND	C3-N2	-2.59	1.33	1.39
2	B	900	3ND	C18-C17	-2.36	1.48	1.51
2	D	900	3ND	C3-N2	-2.30	1.34	1.39
2	B	900	3ND	C3-N2	-2.25	1.34	1.39
2	C	900	3ND	C1-N2	7.14	1.35	1.27

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	3ND	C18-C17-C13	-5.89	100.92	114.54
2	D	900	3ND	C18-C17-C13	-5.61	101.57	114.54
2	C	900	3ND	C18-C17-C13	-5.14	102.64	114.54
2	C	900	3ND	C5-C6-C3	-4.85	118.25	120.87
2	D	900	3ND	C5-C6-C3	-4.74	118.31	120.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	3ND	7	0
2	C	900	3ND	4	0
2	D	900	3ND	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	383/415 (92%)	0.78	61 (15%) 3 2	102, 200, 300, 366	0
1	B	396/415 (95%)	0.19	14 (3%) 48 40	83, 143, 237, 329	0
1	C	371/415 (89%)	0.47	38 (10%) 9 7	88, 168, 274, 403	0
1	D	396/415 (95%)	0.21	9 (2%) 64 57	82, 153, 232, 336	0
All	All	1546/1660 (93%)	0.41	122 (7%) 15 12	82, 164, 271, 403	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	TYR	7.1
1	A	245	VAL	5.2
1	C	260	ASP	5.1
1	A	336	LEU	4.9
1	A	353	ALA	4.8

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	3ND	D	900	27/27	0.88	0.33	0.59	150,150,150,150	0
2	3ND	B	900	27/27	0.90	0.28	0.20	142,142,142,142	0
2	3ND	C	900	27/27	0.92	0.25	-0.62	138,138,138,138	0

6.5 Other polymers (i)

There are no such residues in this entry.