wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 01:11 AM EST

PDB ID	:	3O6B
Title	:	A Dual E3 Mechanism for Rub1 Ligation to Cdc53: Dcn1(P)-Cdc53(WHB) low resolution
Authors	:	Scott, D.C.; Monda, J.K.; Grace, C.R.R.; Duda, D.M.; Kriwacki, R.W.; Kurz, T.; Schulman, B.A.
Deposited on	:	2010-07-28
Resolution	:	3.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

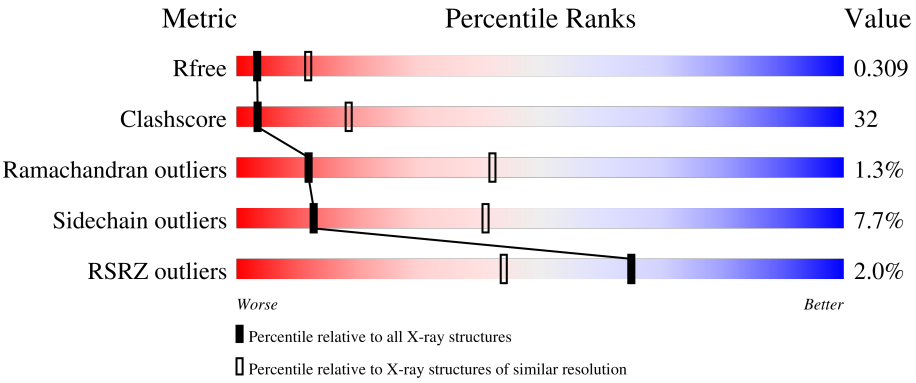
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



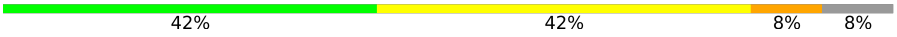
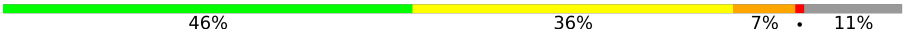
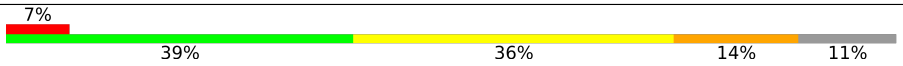
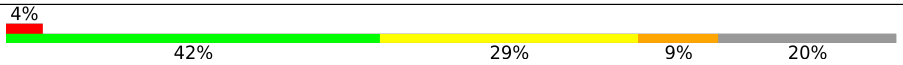
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 >=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.

Mol	Chain	Length	Quality of chain
1	A	202	51% 42%
1	C	202	64% 31%
1	E	202	40% 47% 10%
1	G	202	61% 33% 5%
1	I	202	8% 35% 38% 5% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	76	
2	D	76	
2	F	76	
2	H	76	
2	J	76	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10662 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 Defective in cullin neddylation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1664	1090	256	310	8			
1	C	198	Total	C	N	O	S	0	0	0
			1689	1107	259	315	8			
1	E	195	Total	C	N	O	S	0	0	0
			1667	1094	255	310	8			
1	G	192	Total	C	N	O	S	0	0	0
			1639	1074	251	306	8			
1	I	157	Total	C	N	O	S	0	0	0
			1348	888	208	246	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	-	expression tag	UNP Q12395
A	69	SER	-	expression tag	UNP Q12395
C	68	GLY	-	expression tag	UNP Q12395
C	69	SER	-	expression tag	UNP Q12395
E	68	GLY	-	expression tag	UNP Q12395
E	69	SER	-	expression tag	UNP Q12395
G	68	GLY	-	expression tag	UNP Q12395
G	69	SER	-	expression tag	UNP Q12395
I	68	GLY	-	expression tag	UNP Q12395
I	69	SER	-	expression tag	UNP Q12395

- Molecule 2 is a protein called Cell division control protein 53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	0	0
			559	350	105	100	4			
2	D	68	Total	C	N	O	S	0	0	0
			543	341	99	99	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	68	Total	C	N	O	S	0	0	0
			540	339	97	100	4			
2	H	68	Total	C	N	O	S	0	0	0
			539	339	99	97	4			
2	J	61	Total	C	N	O	S	0	0	0
			474	298	84	88	4			

There are 10 discrepancies between the modelled and reference sequences:

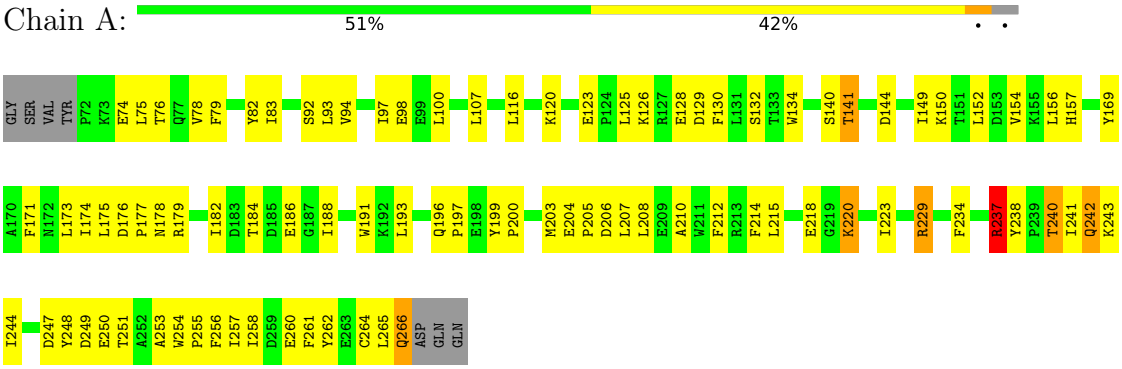
Chain	Residue	Modelled	Actual	Comment	Reference
B	740	GLY	-	expression tag	UNP Q12018
B	741	SER	-	expression tag	UNP Q12018
D	740	GLY	-	expression tag	UNP Q12018
D	741	SER	-	expression tag	UNP Q12018
F	740	GLY	-	expression tag	UNP Q12018
F	741	SER	-	expression tag	UNP Q12018
H	740	GLY	-	expression tag	UNP Q12018
H	741	SER	-	expression tag	UNP Q12018
J	740	GLY	-	expression tag	UNP Q12018
J	741	SER	-	expression tag	UNP Q12018

3 Residue-property plots (i)

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.

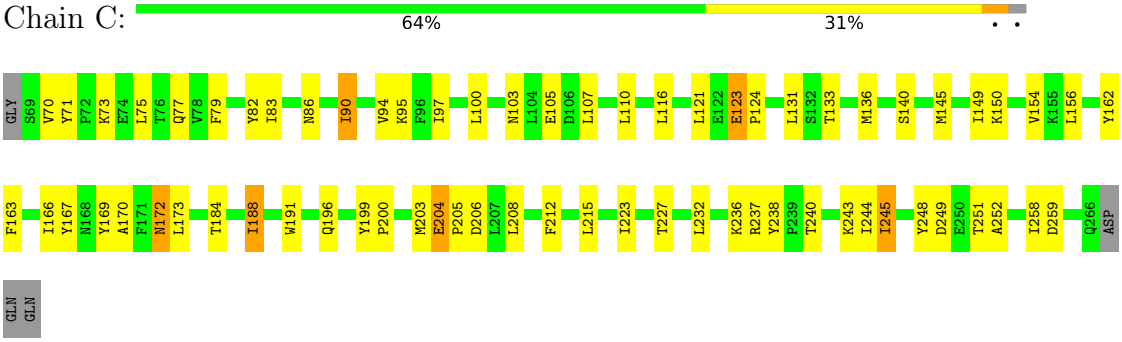
• Molecule 1: Defective in cullin neddylation protein 1

Chain A:



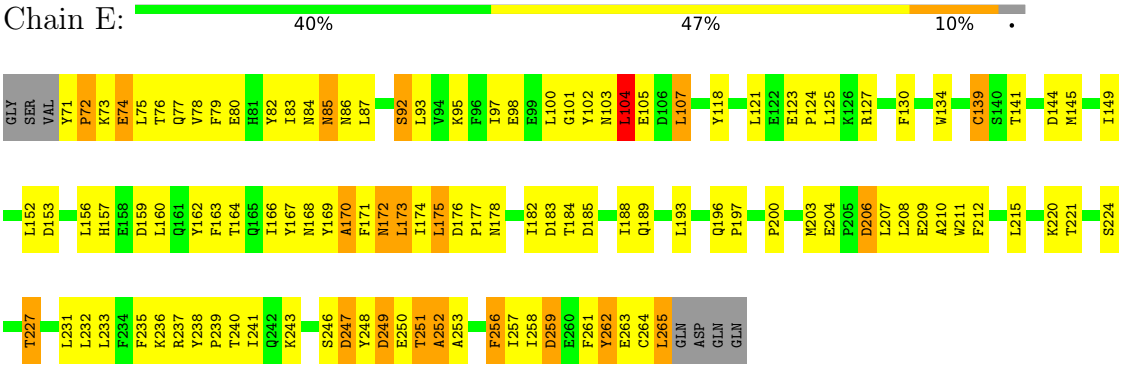
• Molecule 1: Defective in cullin neddylation protein 1

Chain C:



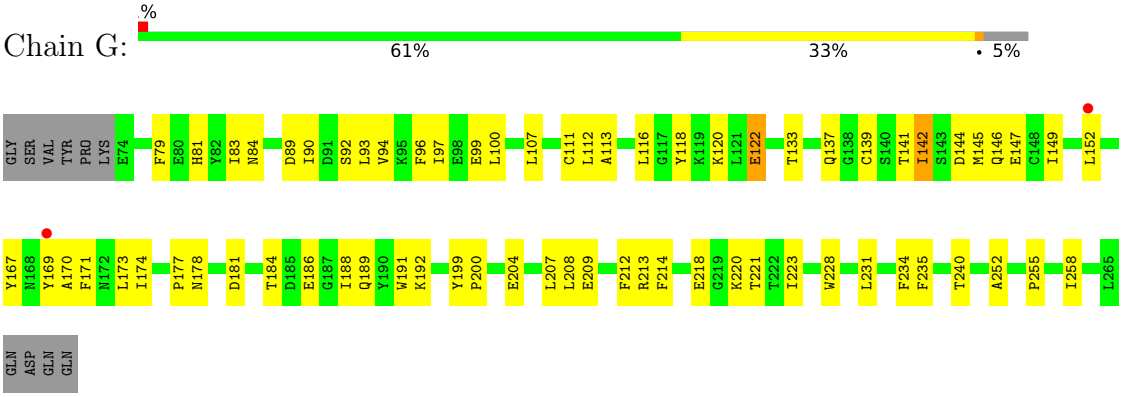
• Molecule 1: Defective in cullin neddylation protein 1

Chain E:



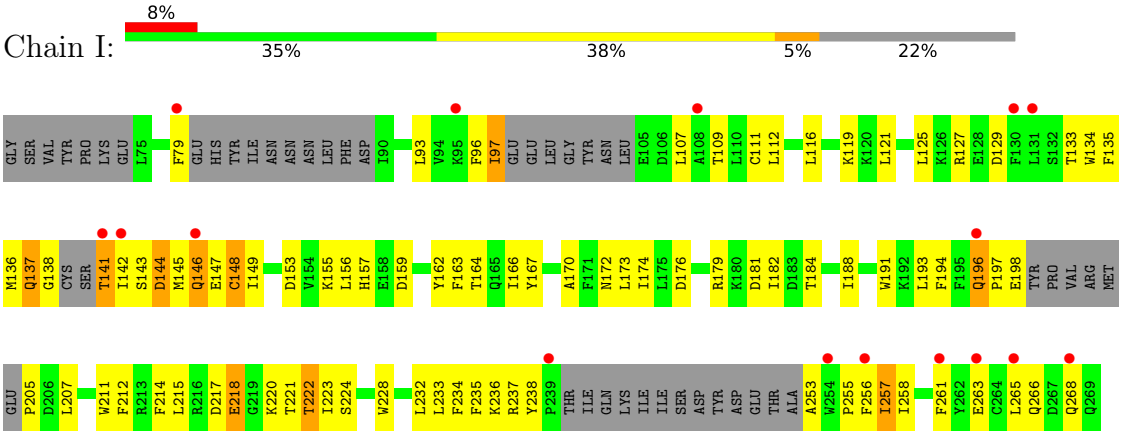
• Molecule 1: Defective in cullin neddylation protein 1

Chain G:



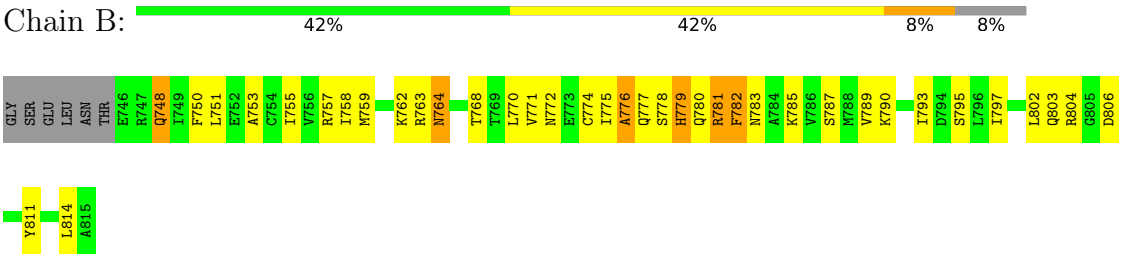
• Molecule 1: Defective in cullin neddylation protein 1

Chain I:



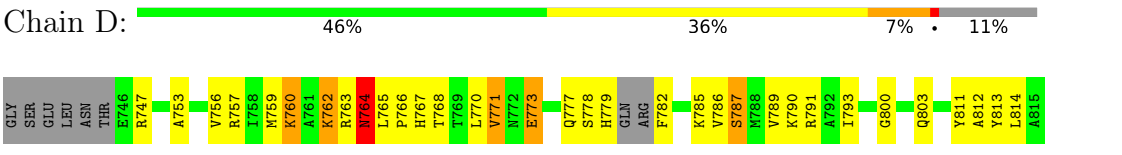
• Molecule 2: Cell division control protein 53

Chain B:



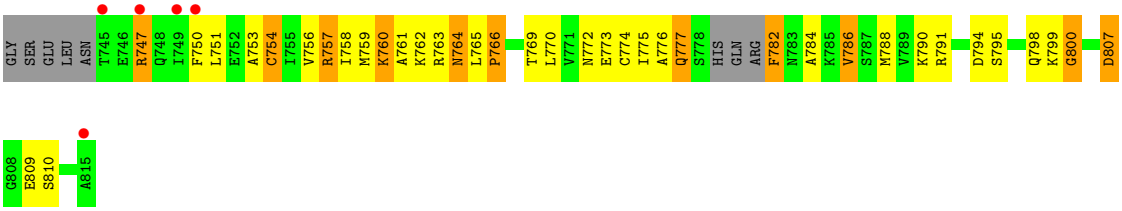
• Molecule 2: Cell division control protein 53

Chain D:

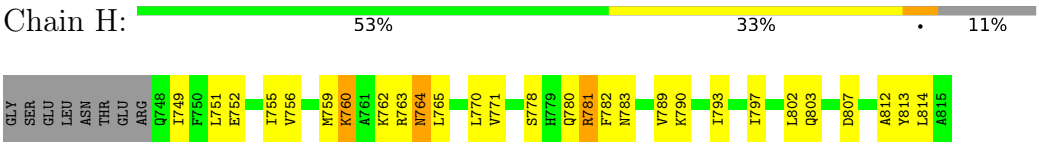


• Molecule 2: Cell division control protein 53

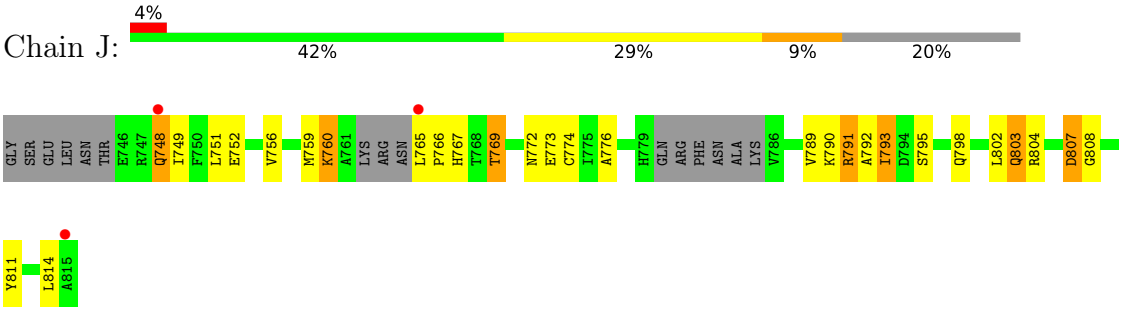
Chain F:



• Molecule 2: Cell division control protein 53



• Molecule 2: Cell division control protein 53



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	123.91Å 123.91Å 192.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 39.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.10) 99.1 (39.69-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.308 0.264 , 0.309	Depositor DCC
R_{free} test set	1532 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10662	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.61	0/1710	0.80	2/2317 (0.1%)
1	C	0.56	0/1736	0.72	0/2354
1	E	0.73	5/1714 (0.3%)	0.81	2/2324 (0.1%)
1	G	0.51	0/1684	0.72	0/2283
1	I	0.46	0/1381	0.71	1/1860 (0.1%)
2	B	0.62	0/566	0.82	0/757
2	D	0.55	0/549	0.70	0/733
2	F	0.50	0/545	0.77	1/728 (0.1%)
2	H	0.56	0/546	0.84	0/731
2	J	0.45	0/478	0.73	1/640 (0.2%)
All	All	0.58	5/10909 (0.0%)	0.76	7/14727 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	170	ALA	C-O	11.32	1.44	1.23
1	E	170	ALA	CA-CB	-6.26	1.39	1.52
1	E	173	LEU	C-O	5.98	1.34	1.23
1	E	172	ASN	C-O	5.98	1.34	1.23
1	E	168	ASN	CG-ND2	5.03	1.45	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	A	237	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
2	F	800	GLY	N-CA-C	5.76	127.50	113.10
1	E	247	ASP	N-CA-C	5.71	126.42	111.00
1	E	253	ALA	N-CA-C	5.61	126.15	111.00

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	A	1664	0	1613	88	3
1	C	1689	0	1635	60	0
1	E	1667	0	1613	150	3
1	G	1639	0	1584	57	0
1	I	1348	0	1311	89	0
2	B	559	0	572	59	0
2	D	543	0	554	57	0
2	F	540	0	554	80	0
2	H	539	0	551	39	0
2	J	474	0	473	29	0
All	All	10662	0	10460	680	3

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 32.

The worst 5 of 680 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)
2:B:758:ILE:HD11	2:B:777:GLN:OE1	1.25	1.24
1:E:71:TYR:HB3	1:E:72:PRO:HD2	1.21	1.17
2:B:779:HIS:CG	2:B:780:GLN:H	1.60	1.15
2:D:762:LYS:HD2	2:D:765:LEU:HD11	1.24	1.15
1:E:261:PHE:O	1:E:265:LEU:HD11	1.47	1.15

All (3) 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:A:237:ARG:NH2	1:E:71:TYR:N[2_655]	2.06	0.14
1:A:247:ASP:OD2	1:E:73:LYS:NZ[2_655]	2.07	0.13
1:A:237:ARG:NH2	1:E:71:TYR:CA[2_655]	2.19	0.01

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	193/202 (96%)	171 (89%)	21 (11%)	1 (0%)	29 64
1	C	196/202 (97%)	177 (90%)	18 (9%)	1 (0%)	29 64
1	E	193/202 (96%)	167 (86%)	22 (11%)	4 (2%)	7 30
1	G	190/202 (94%)	172 (90%)	18 (10%)	0	100 100
1	I	145/202 (72%)	128 (88%)	15 (10%)	2 (1%)	11 40
2	B	68/76 (90%)	58 (85%)	6 (9%)	4 (6%)	1 10
2	D	64/76 (84%)	58 (91%)	5 (8%)	1 (2%)	9 37
2	F	64/76 (84%)	57 (89%)	6 (9%)	1 (2%)	9 37
2	H	66/76 (87%)	60 (91%)	6 (9%)	0	100 100
2	J	55/76 (72%)	48 (87%)	5 (9%)	2 (4%)	3 20
All	All	1234/1390 (89%)	1096 (89%)	122 (10%)	16 (1%)	12 42

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	764	ASN
2	B	779	HIS
2	B	782	PHE
2	D	764	ASN
1	E	72	PRO

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	184/190 (97%)	174 (95%)	10 (5%)	22 53
1	C	187/190 (98%)	176 (94%)	11 (6%)	19 50
1	E	184/190 (97%)	167 (91%)	17 (9%)	9 33
1	G	181/190 (95%)	177 (98%)	4 (2%)	52 78
1	I	148/190 (78%)	131 (88%)	17 (12%)	5 22
2	B	59/65 (91%)	53 (90%)	6 (10%)	7 27
2	D	58/65 (89%)	51 (88%)	7 (12%)	5 20
2	F	58/65 (89%)	48 (83%)	10 (17%)	2 9
2	H	57/65 (88%)	54 (95%)	3 (5%)	22 54
2	J	50/65 (77%)	45 (90%)	5 (10%)	7 28
All	All	1166/1275 (92%)	1076 (92%)	90 (8%)	13 41

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	782	PHE
1	I	144	ASP
2	F	794	ASP
2	H	760	LYS
1	I	205	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	764	ASN
2	J	798	GLN
1	G	84	ASN
1	I	172	ASN
1	G	81	HIS

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 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^{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	195/202 (96%)	-0.07	0 100 100	67, 93, 113, 129	0
1	C	198/202 (98%)	-0.05	0 100 100	66, 88, 118, 133	0
1	E	195/202 (96%)	-0.01	0 100 100	80, 118, 139, 144	0
1	G	192/202 (95%)	0.00	2 (1%) 82 67	79, 113, 137, 145	0
1	I	157/202 (77%)	0.58	16 (10%) 6 2	135, 153, 179, 191	0
2	B	70/76 (92%)	0.01	0 100 100	80, 103, 141, 149	0
2	D	68/76 (89%)	-0.02	0 100 100	80, 110, 135, 150	0
2	F	68/76 (89%)	0.24	5 (7%) 14 5	106, 129, 157, 163	0
2	H	68/76 (89%)	-0.01	0 100 100	89, 111, 129, 136	0
2	J	61/76 (80%)	0.33	3 (4%) 29 14	116, 135, 154, 156	0
All	All	1272/1390 (91%)	0.08	26 (2%) 65 44	66, 111, 159, 191	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	265	LEU	6.9
1	I	239	PRO	5.5
1	I	141	THR	4.1
1	I	146	GLN	3.6
2	F	745	THR	3.3

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 (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.