



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2017 – 10:16 PM EDT

PDB ID : 3WHL  
Title : Crystal structure of Nas2 N-terminal domain complexed with PAN-Rpt5C chimera  
Authors : Satoh, T.; Saeki, Y.; Hiromoto, T.; Wang, Y.-H.; Uekusa, Y.; Yagi, H.; Yoshihara, H.; Yagi-Utsumi, M.; Mizushima, T.; Tanaka, K.; Kato, K.  
Deposited on : unknown  
Resolution : 4.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

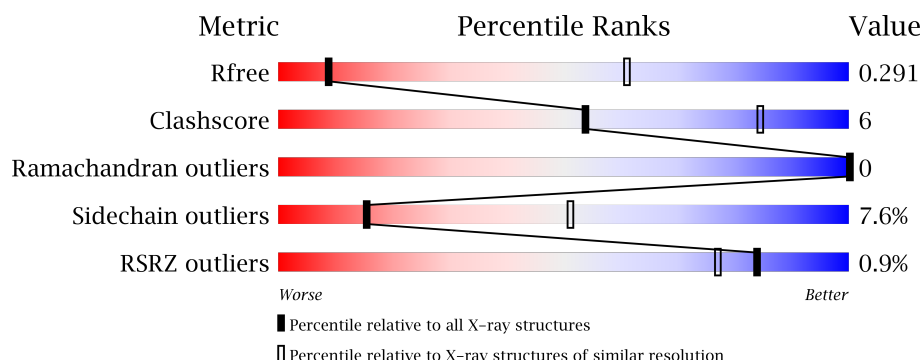
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	270	
1	C	270	
1	E	270	
1	G	270	
2	B	122	

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Mol	Chain	Length	Quality of chain
2	D	122	
2	F	122	
2	H	122	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10333 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 Proteasome-activating nucleotidase, 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1855	1175	324	350	6			
1	C	232	Total	C	N	O	S	0	0	0
			1813	1150	319	338	6			
1	E	228	Total	C	N	O	S	0	0	0
			1789	1138	313	332	6			
1	G	234	Total	C	N	O	S	0	0	0
			1828	1160	320	342	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLY	-	EXPRESSION TAG	UNP Q8U4H3
A	166	SER	-	EXPRESSION TAG	UNP Q8U4H3
A	167	HIS	-	EXPRESSION TAG	UNP Q8U4H3
A	168	MET	-	EXPRESSION TAG	UNP Q8U4H3
A	354	GLU	-	LINKER	UNP P33297
A	355	PHE	-	LINKER	UNP P33297
C	165	GLY	-	EXPRESSION TAG	UNP Q8U4H3
C	166	SER	-	EXPRESSION TAG	UNP Q8U4H3
C	167	HIS	-	EXPRESSION TAG	UNP Q8U4H3
C	168	MET	-	EXPRESSION TAG	UNP Q8U4H3
C	354	GLU	-	LINKER	UNP P33297
C	355	PHE	-	LINKER	UNP P33297
E	165	GLY	-	EXPRESSION TAG	UNP Q8U4H3
E	166	SER	-	EXPRESSION TAG	UNP Q8U4H3
E	167	HIS	-	EXPRESSION TAG	UNP Q8U4H3
E	168	MET	-	EXPRESSION TAG	UNP Q8U4H3
E	354	GLU	-	LINKER	UNP P33297
E	355	PHE	-	LINKER	UNP P33297
G	165	GLY	-	EXPRESSION TAG	UNP Q8U4H3
G	166	SER	-	EXPRESSION TAG	UNP Q8U4H3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	167	HIS	-	EXPRESSION TAG	UNP Q8U4H3
G	168	MET	-	EXPRESSION TAG	UNP Q8U4H3
G	354	GLU	-	LINKER	UNP P33297
G	355	PHE	-	LINKER	UNP P33297

- Molecule 2 is a protein called Probable 26S proteasome regulatory subunit p27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			737	463	126	143	5			
2	D	92	Total	C	N	O	S	0	0	0
			737	463	126	143	5			
2	F	90	Total	C	N	O	S	0	0	0
			721	454	124	139	4			
2	H	91	Total	C	N	O	S	0	0	0
			729	460	125	140	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP P40555
B	0	SER	-	EXPRESSION TAG	UNP P40555
D	-1	GLY	-	EXPRESSION TAG	UNP P40555
D	0	SER	-	EXPRESSION TAG	UNP P40555
F	-1	GLY	-	EXPRESSION TAG	UNP P40555
F	0	SER	-	EXPRESSION TAG	UNP P40555
H	-1	GLY	-	EXPRESSION TAG	UNP P40555
H	0	SER	-	EXPRESSION TAG	UNP P40555

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

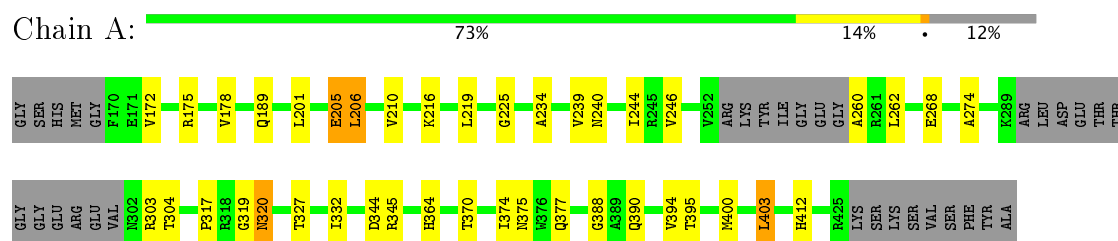


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

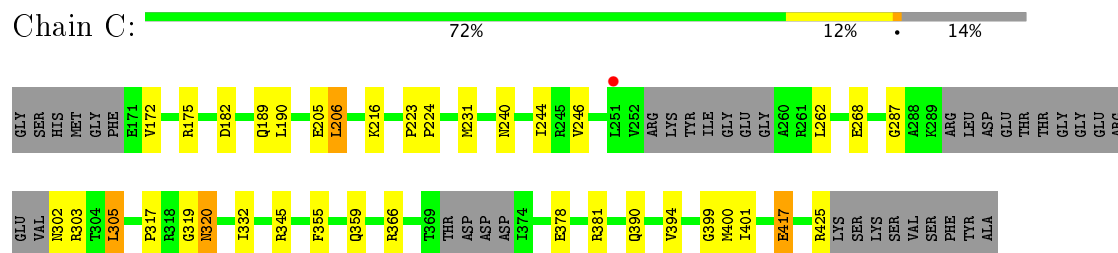
### 3 Residue-property plots

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.

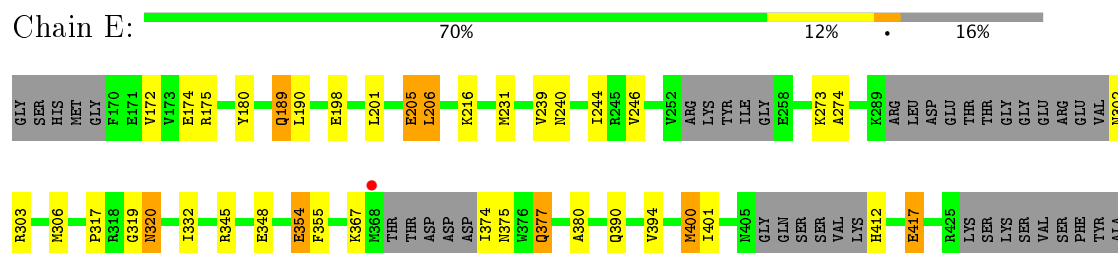
- Molecule 1: Proteasome-activating nucleotidase, 26S protease regulatory subunit 6A



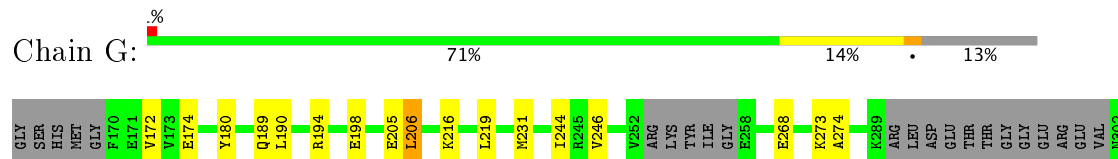
- Molecule 1: Proteasome-activating nucleotidase, 26S protease regulatory subunit 6A

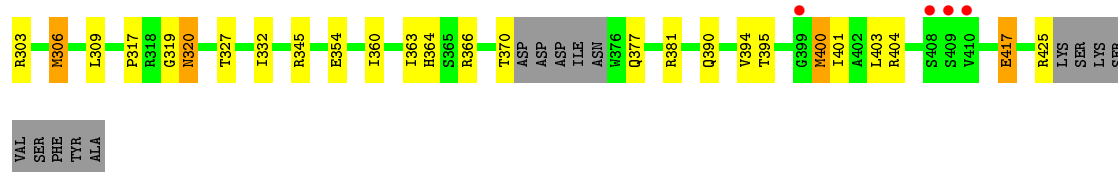


- Molecule 1: Proteasome-activating nucleotidase, 26S protease regulatory subunit 6A

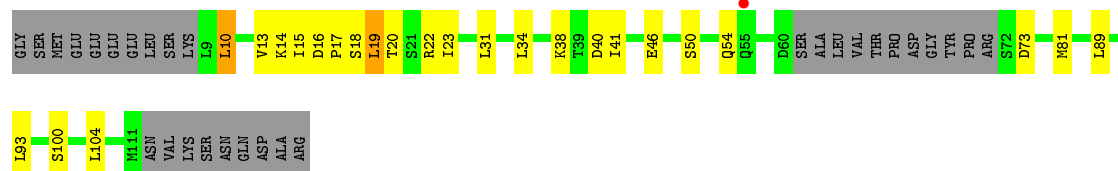


- Molecule 1: Proteasome-activating nucleotidase, 26S protease regulatory subunit 6A





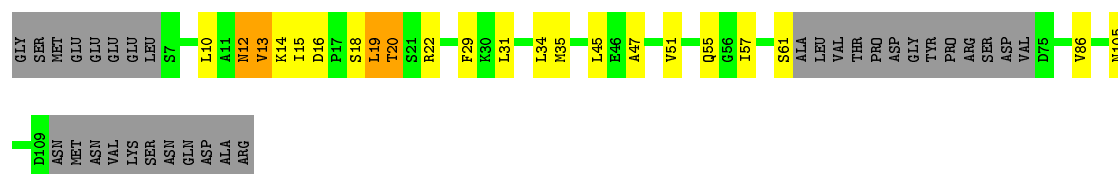
- Molecule 2: Probable 26S proteasome regulatory subunit p27



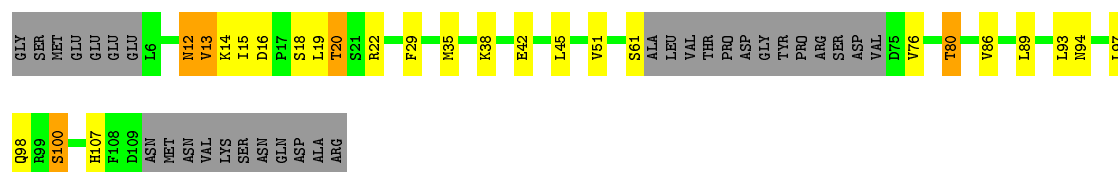
- Molecule 2: Probable 26S proteasome regulatory subunit p27



- Molecule 2: Probable 26S proteasome regulatory subunit p27



- Molecule 2: Probable 26S proteasome regulatory subunit p27





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.63Å 110.63Å 251.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 4.00 38.46 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.94-4.00) 99.4 (38.46-4.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.38 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.233 , 0.285 0.235 , 0.291	Depositor DCC
$R_{free}$ test set	774 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	138.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 92.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: ATP

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	0.23	0/1885	0.43	0/2548
1	C	0.23	0/1841	0.44	0/2486
1	E	0.23	0/1817	0.44	0/2452
1	G	0.23	0/1857	0.44	0/2507
2	B	0.24	0/743	0.44	0/1000
2	D	0.27	0/743	0.47	0/1000
2	F	0.24	0/727	0.49	0/977
2	H	0.24	0/735	0.52	0/988
All	All	0.24	0/10348	0.45	0/13958

There are no bond length outliers.

There are no bond angle outliers.

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	1855	0	1879	21	0
1	C	1813	0	1850	18	0
1	E	1789	0	1817	23	0
1	G	1828	0	1858	23	0
2	B	737	0	752	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	737	0	752	13	0
2	F	721	0	742	12	0
2	H	729	0	753	17	0
3	A	31	0	12	0	0
3	C	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	1	0
All	All	10333	0	10451	127	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 6.

All (127) 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:C:206:LEU:HD22	1:E:206:LEU:HD22	1.70	0.72
2:D:10:LEU:HD11	2:D:13:VAL:HB	1.72	0.71
1:G:216:LYS:HE2	1:G:317:PRO:HD3	1.74	0.70
1:A:210:VAL:O	1:G:194:ARG:NH2	2.25	0.69
2:F:14:LYS:HD3	2:F:47:ALA:HB1	1.73	0.68
1:C:216:LYS:HE2	1:C:317:PRO:HD3	1.77	0.67
1:A:206:LEU:HD22	1:G:206:LEU:HD22	1.78	0.66
2:F:19:LEU:HD13	2:F:22:ARG:HD2	1.79	0.65
1:C:425:ARG:NH2	2:D:42:GLU:OE2	2.29	0.65
2:D:16:ASP:HB3	2:D:19:LEU:HB2	1.77	0.65
1:E:375:ASN:OD1	1:E:377:GLN:HG2	1.97	0.65
2:F:12:ASN:OD1	2:F:12:ASN:N	2.30	0.63
2:D:22:ARG:NH2	2:D:40:ASP:OD2	2.31	0.61
2:H:12:ASN:N	2:H:12:ASN:OD1	2.33	0.61
1:C:401:ILE:HD13	1:C:417:GLU:HG2	1.83	0.60
1:G:401:ILE:HD13	1:G:417:GLU:HG2	1.82	0.60
2:B:16:ASP:HB3	2:B:19:LEU:HB2	1.85	0.59
1:E:374:ILE:HG12	1:E:412:HIS:HB2	1.83	0.59
1:A:216:LYS:HE2	1:A:317:PRO:HD3	1.84	0.59
1:E:175:ARG:NH1	1:E:240:ASN:OD1	2.38	0.57
1:C:378:GLU:HG3	1:C:381:ARG:NH2	2.20	0.57
1:C:287:GLY:HA2	1:C:305:LEU:HD22	1.87	0.57
2:H:35:MET:HA	2:H:35:MET:HE2	1.86	0.56
2:H:76:VAL:O	2:H:80:THR:OG1	2.22	0.56
1:E:216:LYS:HE2	1:E:317:PRO:HD3	1.88	0.55
2:H:18:SER:C	2:H:20:THR:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:HD13	2:B:23:ILE:HG13	1.89	0.55
1:E:180:TYR:OH	1:E:198:GLU:OE1	2.24	0.54
1:A:364:HIS:HB2	1:A:395:THR:HG21	1.89	0.54
1:G:425:ARG:NH2	2:H:42:GLU:OE2	2.40	0.54
1:C:175:ARG:NH1	1:C:240:ASN:OD1	2.40	0.54
2:H:38:LYS:HG3	2:H:93:LEU:HD11	1.89	0.53
2:F:13:VAL:HG13	2:F:51:VAL:HG21	1.91	0.53
1:C:175:ARG:HD3	1:C:240:ASN:HA	1.92	0.52
2:D:10:LEU:HD22	2:D:51:VAL:HG21	1.93	0.51
1:G:274:ALA:HB1	1:G:320:ASN:OD1	2.10	0.51
2:F:18:SER:C	2:F:20:THR:H	2.14	0.51
1:G:400:MET:HG2	2:H:35:MET:SD	2.52	0.50
1:A:375:ASN:OD1	1:A:377:GLN:HG2	2.11	0.50
1:E:274:ALA:HB1	1:E:320:ASN:OD1	2.11	0.50
1:A:201:LEU:HD23	1:A:239:VAL:HG21	1.92	0.50
1:E:401:ILE:HD13	1:E:417:GLU:HG2	1.93	0.50
1:A:205:GLU:OE1	1:A:206:LEU:N	2.45	0.49
2:F:55:GLN:HB2	2:F:57:ILE:HG22	1.94	0.49
1:A:172:VAL:HG22	1:A:244:ILE:HG23	1.94	0.49
1:C:355:PHE:CD1	1:G:354:GLU:HG2	2.46	0.49
2:B:15:ILE:O	2:B:17:PRO:HD3	2.13	0.49
2:D:76:VAL:O	2:D:80:THR:OG1	2.23	0.49
1:E:172:VAL:HG22	1:E:244:ILE:HG23	1.93	0.49
1:A:175:ARG:HD3	1:A:240:ASN:HA	1.94	0.48
1:A:260:ALA:N	1:A:304:THR:HG1	2.11	0.48
1:A:320:ASN:H	1:A:320:ASN:HD22	1.61	0.48
2:B:22:ARG:NH2	2:B:40:ASP:OD2	2.41	0.48
1:G:317:PRO:C	1:G:319:GLY:H	2.17	0.48
2:H:13:VAL:O	2:H:14:LYS:HG3	2.13	0.48
1:A:374:ILE:HG12	1:A:412:HIS:HB2	1.95	0.48
1:E:367:LYS:HE3	2:F:105:ASN:HB3	1.95	0.48
2:H:13:VAL:HG12	2:H:14:LYS:N	2.29	0.48
1:E:390:GLN:O	1:E:394:VAL:HG23	2.13	0.47
1:E:320:ASN:HD22	1:E:320:ASN:H	1.63	0.47
1:C:190:LEU:HD13	1:C:231:MET:HG2	1.96	0.47
1:C:399:GLY:HA3	2:D:104:LEU:HD21	1.96	0.47
1:C:390:GLN:O	1:C:394:VAL:HG23	2.13	0.47
1:G:174:GLU:OE2	1:G:273:LYS:NZ	2.37	0.47
2:D:23:ILE:HD12	2:D:92:ASP:HB3	1.95	0.47
1:C:359:GLN:OE1	1:G:381:ARG:NH2	2.48	0.47
2:B:13:VAL:HG13	2:B:14:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:HG13	1:A:244:ILE:HG12	1.97	0.47
2:H:94:ASN:O	2:H:98:GLN:HG2	2.14	0.47
1:A:274:ALA:HB1	1:A:320:ASN:OD1	2.16	0.46
1:G:320:ASN:HD22	1:G:320:ASN:H	1.64	0.46
1:C:172:VAL:HG22	1:C:244:ILE:HG23	1.97	0.46
1:E:205:GLU:OE1	1:E:206:LEU:N	2.49	0.46
1:E:400:MET:HG3	2:F:35:MET:SD	2.56	0.46
2:B:41:ILE:HG23	2:B:89:LEU:HD22	1.98	0.45
2:F:31:LEU:HD23	2:F:34:LEU:HD12	1.98	0.45
1:A:317:PRO:C	1:A:319:GLY:H	2.20	0.45
2:D:41:ILE:HG23	2:D:89:LEU:HD22	1.98	0.45
1:G:360:ILE:HG12	3:G:600:ATP:N1	2.32	0.45
2:D:107:HIS:O	2:D:111:MET:HG3	2.17	0.45
2:H:22:ARG:HB3	2:H:29:PHE:HE2	1.82	0.44
2:H:45:LEU:HD22	2:H:86:VAL:HG13	2.00	0.44
2:B:100:SER:O	2:B:104:LEU:HB2	2.17	0.44
1:G:172:VAL:HG22	1:G:244:ILE:HG23	1.99	0.44
1:A:225:GLY:O	1:A:388:GLY:N	2.49	0.44
1:E:175:ARG:HD3	1:E:240:ASN:HA	1.99	0.44
1:C:320:ASN:HD22	1:C:320:ASN:H	1.65	0.44
1:G:363:ILE:HG12	1:G:366:ARG:NH2	2.33	0.44
1:E:354:GLU:HG3	1:E:354:GLU:H	1.40	0.44
1:C:182:ASP:OD1	1:C:366:ARG:NH1	2.51	0.43
1:E:201:LEU:HD23	1:E:239:VAL:HG21	2.00	0.43
1:A:219:LEU:HD11	1:A:327:THR:HG22	2.00	0.43
2:D:19:LEU:HD22	2:D:23:ILE:HG12	2.00	0.43
1:G:180:TYR:OH	1:G:198:GLU:OE1	2.35	0.43
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.75	0.43
2:B:50:SER:O	2:B:54:GLN:HG3	2.19	0.43
2:D:100:SER:O	2:D:104:LEU:HB2	2.19	0.43
1:E:375:ASN:H	1:E:412:HIS:CD2	2.37	0.43
2:D:13:VAL:HG13	2:D:14:LYS:O	2.18	0.43
1:E:174:GLU:OE2	1:E:273:LYS:NZ	2.32	0.43
2:H:13:VAL:HG13	2:H:51:VAL:HG21	2.00	0.43
2:F:13:VAL:HG12	2:F:14:LYS:N	2.34	0.43
1:G:219:LEU:HD11	1:G:327:THR:HG22	2.01	0.43
2:H:19:LEU:HB3	2:H:22:ARG:HD2	2.01	0.43
1:C:317:PRO:C	1:C:319:GLY:H	2.23	0.42
1:G:364:HIS:HB2	1:G:395:THR:HG21	2.01	0.42
1:G:306:MET:HA	1:G:309:LEU:HD12	2.02	0.42
2:H:97:LEU:HA	2:H:100:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLN:O	1:A:394:VAL:HG23	2.20	0.42
1:A:178:VAL:O	1:A:234:ALA:HA	2.21	0.41
2:H:89:LEU:HD23	2:H:89:LEU:HA	1.88	0.41
1:E:189:GLN:NE2	1:E:348:GLU:O	2.52	0.41
1:E:190:LEU:HD13	1:E:231:MET:HG2	2.01	0.41
2:F:45:LEU:HD22	2:F:86:VAL:HG13	2.03	0.41
2:B:31:LEU:HD23	2:B:34:LEU:HD12	2.03	0.41
1:E:317:PRO:C	1:E:319:GLY:H	2.23	0.41
1:E:354:GLU:O	1:E:380:ALA:HB1	2.21	0.41
1:G:403:LEU:HD23	1:G:403:LEU:HA	1.90	0.41
2:B:10:LEU:CD1	2:B:13:VAL:HB	2.51	0.41
1:G:190:LEU:HD13	1:G:231:MET:HG2	2.03	0.41
1:G:404:ARG:NH1	2:H:35:MET:SD	2.94	0.41
2:B:38:LYS:HG3	2:B:93:LEU:HD11	2.03	0.41
2:B:10:LEU:HD11	2:B:13:VAL:HB	2.03	0.40
2:F:22:ARG:HB3	2:F:29:PHE:HE2	1.86	0.40
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.93	0.40
1:G:390:GLN:O	1:G:394:VAL:HG23	2.20	0.40
1:A:344:ASP:N	1:A:344:ASP:OD2	2.53	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	231/270 (86%)	223 (96%)	8 (4%)	0	100	100
1	C	224/270 (83%)	216 (96%)	8 (4%)	0	100	100
1	E	218/270 (81%)	208 (95%)	10 (5%)	0	100	100
1	G	226/270 (84%)	216 (96%)	10 (4%)	0	100	100
2	B	88/122 (72%)	85 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	88/122 (72%)	86 (98%)	2 (2%)	0	100	100
2	F	86/122 (70%)	84 (98%)	2 (2%)	0	100	100
2	H	87/122 (71%)	83 (95%)	4 (5%)	0	100	100
All	All	1248/1568 (80%)	1201 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	200/226 (88%)	187 (94%)	13 (6%)	20	56
1	C	195/226 (86%)	181 (93%)	14 (7%)	17	53
1	E	191/226 (84%)	176 (92%)	15 (8%)	14	49
1	G	196/226 (87%)	182 (93%)	14 (7%)	17	53
2	B	88/114 (77%)	81 (92%)	7 (8%)	14	49
2	D	88/114 (77%)	82 (93%)	6 (7%)	18	55
2	F	86/114 (75%)	78 (91%)	8 (9%)	10	42
2	H	87/114 (76%)	78 (90%)	9 (10%)	8	37
All	All	1131/1360 (83%)	1045 (92%)	86 (8%)	15	51

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	205	GLU
1	A	206	LEU
1	A	246	VAL
1	A	262	LEU
1	A	268	GLU
1	A	303	ARG
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	332	ILE
1	A	345	ARG
1	A	370	THR
1	A	400	MET
1	A	403	LEU
2	B	10	LEU
2	B	18	SER
2	B	19	LEU
2	B	20	THR
2	B	46	GLU
2	B	73	ASP
2	B	81	MET
1	C	189	GLN
1	C	205	GLU
1	C	206	LEU
1	C	246	VAL
1	C	262	LEU
1	C	268	GLU
1	C	302	ASN
1	C	303	ARG
1	C	305	LEU
1	C	320	ASN
1	C	332	ILE
1	C	345	ARG
1	C	400	MET
1	C	417	GLU
2	D	10	LEU
2	D	19	LEU
2	D	46	GLU
2	D	73	ASP
2	D	81	MET
2	D	100	SER
1	E	189	GLN
1	E	205	GLU
1	E	206	LEU
1	E	246	VAL
1	E	302	ASN
1	E	303	ARG
1	E	306	MET
1	E	320	ASN
1	E	332	ILE
1	E	345	ARG

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Mol	Chain	Res	Type
1	E	354	GLU
1	E	355	PHE
1	E	377	GLN
1	E	400	MET
1	E	417	GLU
2	F	10	LEU
2	F	12	ASN
2	F	13	VAL
2	F	15	ILE
2	F	16	ASP
2	F	19	LEU
2	F	20	THR
2	F	61	SER
1	G	189	GLN
1	G	205	GLU
1	G	206	LEU
1	G	246	VAL
1	G	268	GLU
1	G	303	ARG
1	G	306	MET
1	G	320	ASN
1	G	332	ILE
1	G	345	ARG
1	G	370	THR
1	G	377	GLN
1	G	400	MET
1	G	417	GLU
2	H	12	ASN
2	H	13	VAL
2	H	15	ILE
2	H	16	ASP
2	H	20	THR
2	H	61	SER
2	H	80	THR
2	H	100	SER
2	H	107	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	ASN
1	C	407	GLN

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Mol	Chain	Res	Type
1	E	412	HIS
2	F	101	HIS

### 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 ⓘ

4 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	$\# Z  > 2$
3	ATP	A	600	-	27,33,33	0.96	1 (3%)	25,52,52	1.61	2 (8%)
3	ATP	C	600	-	27,33,33	1.00	1 (3%)	25,52,52	1.59	3 (12%)
3	ATP	E	600	-	27,33,33	0.97	1 (3%)	25,52,52	1.60	2 (8%)
3	ATP	G	600	-	27,33,33	0.99	1 (3%)	25,52,52	1.64	2 (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	ATP	A	600	-	-	0/18/38/38	0/3/3/3
3	ATP	C	600	-	-	0/18/38/38	0/3/3/3
3	ATP	E	600	-	-	0/18/38/38	0/3/3/3
3	ATP	G	600	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	ATP	C5-C4	3.04	1.47	1.40
3	E	600	ATP	C5-C4	3.11	1.47	1.40
3	G	600	ATP	C5-C4	3.16	1.47	1.40
3	C	600	ATP	C5-C4	3.19	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	600	ATP	N3-C2-N1	-5.95	123.67	128.86
3	E	600	ATP	N3-C2-N1	-5.81	123.80	128.86
3	C	600	ATP	N3-C2-N1	-5.65	123.94	128.86
3	A	600	ATP	N3-C2-N1	-5.60	123.98	128.86
3	G	600	ATP	C4-C5-N7	-2.86	106.65	109.41
3	E	600	ATP	C4-C5-N7	-2.78	106.72	109.41
3	A	600	ATP	C4-C5-N7	-2.78	106.73	109.41
3	C	600	ATP	C4-C5-N7	-2.74	106.76	109.41
3	C	600	ATP	C4'-O4'-C1'	2.06	111.96	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	600	ATP	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	237/270 (87%)	-0.23	0 100 100	104, 141, 173, 203	0
1	C	232/270 (85%)	-0.08	1 (0%) 92 88	106, 143, 175, 204	0
1	E	228/270 (84%)	-0.16	1 (0%) 92 88	104, 143, 176, 202	0
1	G	234/270 (86%)	-0.04	4 (1%) 70 61	109, 144, 181, 218	0
2	B	92/122 (75%)	-0.01	1 (1%) 80 72	119, 154, 188, 205	0
2	D	92/122 (75%)	0.04	5 (5%) 26 21	124, 158, 190, 203	0
2	F	90/122 (73%)	-0.14	0 100 100	126, 158, 188, 202	0
2	H	91/122 (74%)	0.14	0 100 100	124, 157, 185, 199	0
All	All	1296/1568 (82%)	-0.09	12 (0%) 84 77	104, 147, 182, 218	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	59	MET	3.4
2	B	55	GLN	3.4
1	G	408	SER	3.2
2	D	55	GLN	3.2
2	D	54	GLN	3.0
1	G	399	GLY	2.9
2	D	58	GLY	2.4
1	G	410	VAL	2.3
2	D	51	VAL	2.2
1	C	251	LEU	2.1
1	E	368	MET	2.0
1	G	409	SER	2.0

## 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](#)

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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	A	600	31/31	0.91	0.28	0.57	96,116,153,168	0
3	ATP	G	600	31/31	0.86	0.31	0.53	102,126,153,169	0
3	ATP	E	600	31/31	0.90	0.25	0.22	99,133,156,164	0
3	ATP	C	600	31/31	0.94	0.20	-0.71	106,121,161,176	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.