



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:17 PM GMT

PDB ID : 3AJI  
Title : Structure of Gankyrin-S6ATPase photo-cross-linked site-specifically, and incorporated by genetic code expansion  
Authors : Sato, S.; Mimasu, S.; Sato, A.; Hino, N.; Sakamoto, K.; Umehara, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2010-06-07  
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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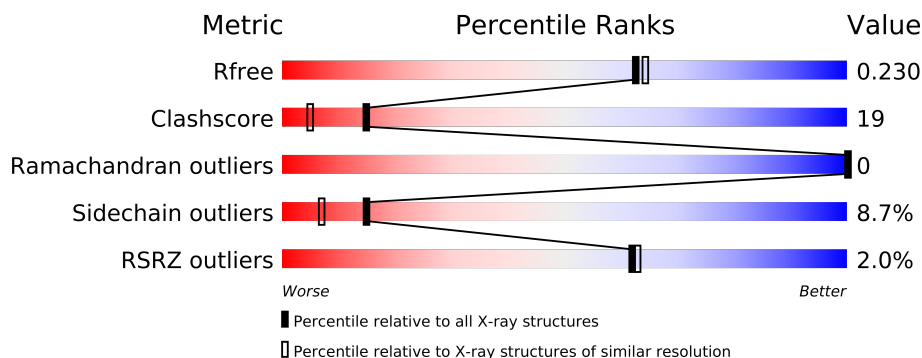
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.05 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))
$R_{free}$	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	231	
1	C	231	
2	B	83	
2	D	83	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4995 atoms, of which 0 are hydrogen and 0 are deuterium.

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 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1745	1092	306	337	10			
1	C	229	Total	C	N	O	S	0	0	0
			1745	1092	306	337	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	PBF	ARG	ENGINEERED MUTATION	UNP Q9Z2X2
C	85	PBF	ARG	ENGINEERED MUTATION	UNP Q9Z2X2

- Molecule 2 is a protein called Proteasome (Prosome, macropain) 26S subunit, ATPase, 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			
2	D	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	MET	-	EXPRESSION TAG	UNP Q6ZWN9
D	336	MET	-	EXPRESSION TAG	UNP Q6ZWN9

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		
3	B	22	Total	O	0	0
			22	22		

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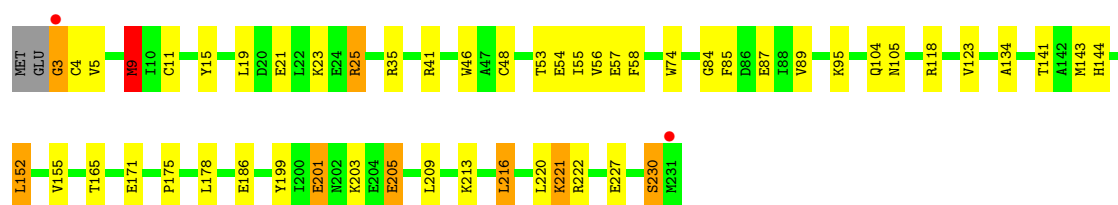
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	142	Total 142	O 142	0	0
3	D	19	Total 19	O 19	0	0

### 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 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.

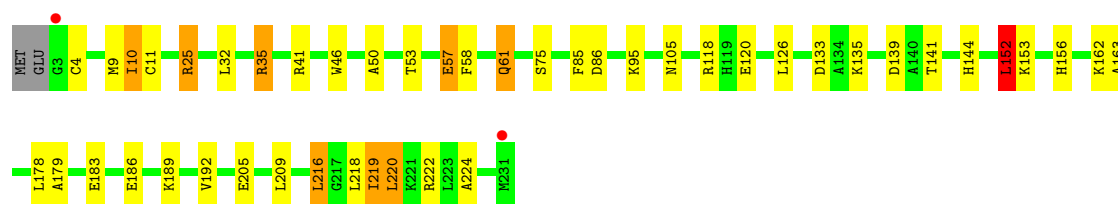
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

Chain A: 



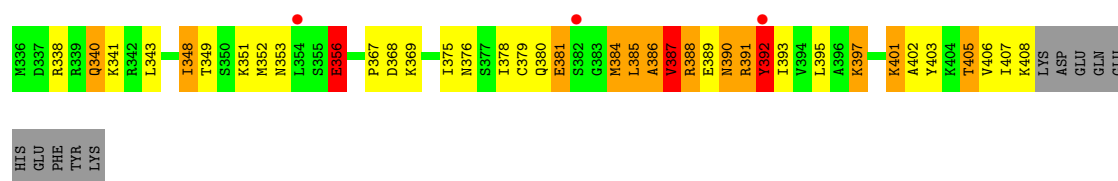
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

Chain C: 



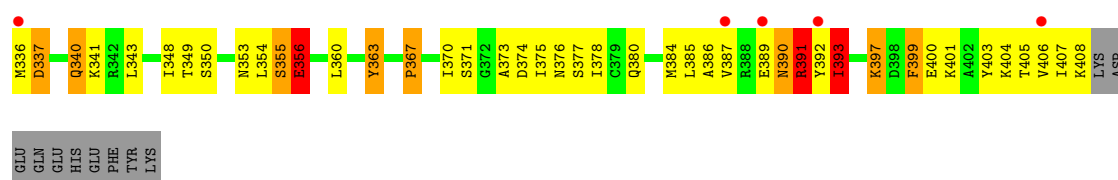
- Molecule 2: Proteasome (Prosome, macropain) 26S subunit, ATPase, 4

Chain B: 



- Molecule 2: Proteasome (Prosome, macropain) 26S subunit, ATPase, 4

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.16Å 103.16Å 154.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.93 – 2.05 42.92 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.93-2.05) 99.9 (42.92-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.05Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.171 , 0.229 0.172 , 0.230	Depositor DCC
$R_{free}$ test set	1914 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.1	EDS
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 38768 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PBF

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	1.49	13/1753 (0.7%)	1.25	10/2368 (0.4%)
1	C	1.48	11/1753 (0.6%)	1.22	12/2368 (0.5%)
2	B	1.39	4/594 (0.7%)	1.58	10/794 (1.3%)
2	D	1.53	5/594 (0.8%)	1.72	13/794 (1.6%)
All	All	1.48	33/4694 (0.7%)	1.35	45/6324 (0.7%)

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
2	B	0	1
2	D	0	2
All	All	0	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	356	GLU	C-N	10.45	1.58	1.34
2	D	356	GLU	CD-OE2	9.96	1.36	1.25
2	B	356	GLU	C-N	9.17	1.55	1.34
2	D	356	GLU	CG-CD	-8.99	1.38	1.51
1	A	205	GLU	CB-CG	7.90	1.67	1.52
1	A	3	GLY	N-CA	7.39	1.57	1.46
1	C	186	GLU	CB-CG	7.31	1.66	1.52
1	A	123	VAL	CB-CG2	7.08	1.67	1.52
1	A	205	GLU	CG-CD	6.72	1.62	1.51
2	D	356	GLU	CD-OE1	6.59	1.32	1.25
1	C	163	ALA	CA-CB	6.42	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ALA	CA-CB	6.31	1.65	1.52
1	A	155	VAL	CB-CG1	6.18	1.65	1.52
1	A	205	GLU	CD-OE1	6.07	1.32	1.25
1	C	25	ARG	CG-CD	-6.01	1.36	1.51
1	C	120	GLU	CG-CD	5.99	1.60	1.51
1	C	224	ALA	CA-CB	5.96	1.65	1.52
1	C	50	ALA	CA-CB	5.93	1.65	1.52
1	A	87	GLU	CB-CG	-5.74	1.41	1.52
2	B	356	GLU	N-CA	5.71	1.57	1.46
1	A	74	TRP	CG-CD1	5.50	1.44	1.36
1	A	54	GLU	CG-CD	5.50	1.60	1.51
2	D	391	ARG	CZ-NH2	5.37	1.40	1.33
1	C	57	GLU	CB-CG	-5.35	1.42	1.52
1	A	56	VAL	CA-CB	5.28	1.65	1.54
1	C	75	SER	CB-OG	-5.26	1.35	1.42
2	B	381	GLU	CG-CD	5.25	1.59	1.51
1	C	179	ALA	CA-CB	5.23	1.63	1.52
1	A	201	GLU	CB-CG	5.22	1.62	1.52
1	C	192	VAL	CB-CG1	5.18	1.63	1.52
1	A	213	LYS	CD-CE	5.13	1.64	1.51
1	C	4	CYS	CB-SG	5.03	1.90	1.82
2	B	341	LYS	CB-CG	-5.02	1.39	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	391	ARG	NE-CZ-NH1	-16.09	112.26	120.30
1	C	25	ARG	NE-CZ-NH1	-10.80	114.90	120.30
2	D	391	ARG	NE-CZ-NH2	10.55	125.57	120.30
2	D	390	ASN	N-CA-C	-10.42	82.86	111.00
1	A	25	ARG	NE-CZ-NH1	-9.88	115.36	120.30
2	D	356	GLU	OE1-CD-OE2	-9.79	111.56	123.30
1	A	9	MET	CG-SD-CE	9.78	115.84	100.20
2	D	356	GLU	CB-CA-C	-9.65	91.10	110.40
1	A	118	ARG	NE-CZ-NH1	-9.47	115.57	120.30
2	D	356	GLU	O-C-N	-9.37	107.70	122.70
2	B	390	ASN	N-CA-C	8.95	135.18	111.00
2	B	387	VAL	N-CA-C	8.95	135.16	111.00
2	B	356	GLU	O-C-N	-8.94	108.40	122.70
2	D	393	ILE	N-CA-C	-8.78	87.30	111.00
1	A	35	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	118	ARG	NE-CZ-NH1	-6.89	116.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	ARG	NE-CZ-NH1	-6.83	116.89	120.30
2	B	356	GLU	N-CA-C	-6.55	93.31	111.00
1	A	4	CYS	N-CA-C	6.50	128.56	111.00
1	C	10	ILE	CB-CG1-CD1	-6.46	95.81	113.90
2	B	386	ALA	CB-CA-C	6.44	119.77	110.10
1	A	25	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	C	86	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	35	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	D	355	SER	O-C-N	6.09	132.45	122.70
2	B	385	LEU	CB-CA-C	-6.05	98.71	110.20
2	B	356	GLU	CA-C-N	6.05	130.50	117.20
2	D	356	GLU	CA-C-N	6.03	130.47	117.20
1	A	152	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	41	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	D	389	GLU	N-CA-C	5.93	127.01	111.00
2	D	355	SER	CA-C-N	-5.87	104.29	117.20
1	C	126	LEU	CA-CB-CG	-5.74	102.11	115.30
1	C	9	MET	CG-SD-CE	-5.65	91.16	100.20
1	C	133	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	25	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	41	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	B	386	ALA	N-CA-C	-5.31	96.67	111.00
1	A	84	GLY	CA-C-O	-5.26	111.12	120.60
2	D	401	LYS	CD-CE-NZ	5.17	123.58	111.70
1	C	152	LEU	CA-CB-CG	5.13	127.11	115.30
2	B	387	VAL	N-CA-CB	-5.11	100.26	111.50
2	D	356	GLU	N-CA-CB	5.08	119.74	110.60
1	C	10	ILE	CA-CB-CG2	5.08	121.05	110.90
1	C	220	LEU	CB-CG-CD1	-5.04	102.42	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
2	B	392	TYR	Sidechain
2	D	363	TYR	Sidechain
2	D	399	PHE	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1731	39	0
1	C	1745	0	1729	31	0
2	B	589	0	604	68	0
2	D	589	0	605	51	0
3	A	144	0	0	3	0
3	B	22	0	0	3	0
3	C	142	0	0	5	1
3	D	19	0	0	2	0
All	All	4995	0	4669	178	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:340:GLN:HE21	2:D:340:GLN:HA	1.11	1.13
2:B:390:ASN:CG	2:B:390:ASN:O	1.84	1.11
2:D:391:ARG:O	2:D:392:TYR:HD2	1.36	1.09
2:D:391:ARG:N	2:D:391:ARG:HE	1.58	1.01
1:C:105:ASN:HB2	3:D:157:HOH:O	1.61	0.99
1:A:205:GLU:HG3	1:A:205:GLU:O	1.63	0.96
2:D:391:ARG:O	2:D:392:TYR:CD2	2.21	0.94
2:D:390:ASN:C	2:D:391:ARG:HE	1.71	0.93
2:B:348:ILE:C	2:B:348:ILE:HD13	1.90	0.92
2:D:363:TYR:OH	2:D:400:GLU:HG2	1.68	0.92
1:C:222:ARG:HH11	1:C:222:ARG:HG2	1.36	0.91
1:A:143:MET:CE	1:A:175:PRO:HG2	2.04	0.88
1:C:57:GLU:O	1:C:61:GLN:HG3	1.73	0.87
1:A:105:ASN:HB3	3:A:314:HOH:O	1.72	0.87
2:B:406:VAL:HG12	2:B:407:ILE:HD12	1.57	0.86
2:D:340:GLN:NE2	2:D:340:GLN:HA	1.89	0.85
1:C:32:LEU:HA	1:C:35:ARG:HD2	1.58	0.84
1:A:143:MET:HE2	1:A:175:PRO:HG2	1.62	0.81
2:B:381:GLU:O	2:B:385:LEU:HD12	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:162:LYS:HE2	3:C:314:HOH:O	1.83	0.79
1:A:85:PBF:HI2	2:B:356:GLU:CD	2.04	0.77
1:C:57:GLU:O	1:C:61:GLN:CG	2.32	0.77
1:C:85:PBF:HI2	2:D:356:GLU:CD	2.05	0.76
2:B:381:GLU:HG3	2:B:385:LEU:HD11	1.67	0.76
2:D:356:GLU:OE2	2:D:356:GLU:HA	1.83	0.76
2:B:353:ASN:HD22	2:B:393:ILE:HA	1.50	0.76
1:C:183:GLU:OE2	3:C:287:HOH:O	2.04	0.76
2:D:407:ILE:O	2:D:408:LYS:HB2	1.86	0.75
2:D:400:GLU:O	2:D:404:LYS:HD3	1.87	0.74
1:C:222:ARG:HH11	1:C:222:ARG:CG	1.99	0.74
1:A:143:MET:HE2	1:A:175:PRO:CG	2.18	0.74
1:A:205:GLU:CG	1:A:205:GLU:O	2.36	0.74
2:B:391:ARG:HH22	2:B:397:LYS:HD3	1.53	0.73
2:D:406:VAL:HG12	2:D:407:ILE:HD12	1.71	0.72
2:B:390:ASN:OD1	2:B:390:ASN:O	2.06	0.72
1:A:105:ASN:ND2	3:A:317:HOH:O	2.22	0.72
1:A:143:MET:HE2	1:A:175:PRO:CB	2.20	0.72
1:A:141:THR:H	1:A:144:HIS:CD2	2.08	0.72
2:B:391:ARG:NH2	2:B:397:LYS:HD3	2.05	0.72
1:C:205:GLU:O	3:C:365:HOH:O	2.08	0.71
1:C:141:THR:H	1:C:144:HIS:CD2	2.09	0.71
2:D:391:ARG:N	2:D:391:ARG:NE	2.39	0.69
1:A:15:TYR:OH	2:B:393:ILE:HD13	1.94	0.68
2:B:387:VAL:HG13	2:B:390:ASN:OD1	1.94	0.68
3:C:316:HOH:O	2:D:397:LYS:HE3	1.94	0.67
2:D:391:ARG:CA	2:D:391:ARG:NE	2.58	0.67
2:B:391:ARG:HD2	2:B:395:LEU:HD11	1.76	0.66
1:A:143:MET:HE1	1:A:175:PRO:HG2	1.77	0.66
2:D:378:ILE:HG13	2:D:406:VAL:HG11	1.77	0.65
1:C:141:THR:OG1	1:C:144:HIS:HD2	1.79	0.65
2:B:381:GLU:O	2:B:385:LEU:CD1	2.43	0.65
2:B:389:GLU:OE2	2:B:391:ARG:NH2	2.29	0.65
2:B:376:ASN:C	2:B:380:GLN:HE21	2.00	0.65
2:B:387:VAL:HA	2:B:390:ASN:HA	1.80	0.64
2:B:391:ARG:NH2	2:B:397:LYS:CD	2.61	0.64
1:A:141:THR:OG1	1:A:144:HIS:HD2	1.81	0.64
1:A:53:THR:O	1:A:57:GLU:HG3	1.97	0.63
2:D:378:ILE:HD11	2:D:407:ILE:HD13	1.80	0.63
2:D:391:ARG:CA	2:D:391:ARG:HE	2.12	0.63
2:B:348:ILE:C	2:B:348:ILE:CD1	2.66	0.63
1:A:216:LEU:HD22	1:A:220:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:381:GLU:HG3	2:B:385:LEU:CD1	2.30	0.62
1:A:186:GLU:HG3	1:C:153:LYS:CD	2.30	0.61
2:B:390:ASN:HB3	3:B:87:HOH:O	2.01	0.61
2:B:407:ILE:O	2:B:407:ILE:HG22	2.01	0.61
2:D:340:GLN:CA	2:D:340:GLN:HE21	1.93	0.61
2:D:390:ASN:C	2:D:391:ARG:NE	2.51	0.60
1:C:61:GLN:NE2	3:C:319:HOH:O	2.33	0.60
2:B:407:ILE:O	2:B:408:LYS:HB2	2.00	0.60
2:B:391:ARG:HH22	2:B:397:LYS:CD	2.15	0.59
2:B:378:ILE:HD11	2:B:407:ILE:HD13	1.84	0.59
1:C:216:LEU:HD22	1:C:220:LEU:HG	1.84	0.59
1:A:15:TYR:HE2	2:B:392:TYR:HH	1.50	0.59
2:B:384:MET:O	2:B:387:VAL:HG23	2.02	0.59
2:B:392:TYR:H	2:B:392:TYR:HD1	1.50	0.59
1:A:186:GLU:HG3	1:C:153:LYS:HD2	1.85	0.58
2:B:392:TYR:N	2:B:392:TYR:CD1	2.68	0.58
2:B:348:ILE:O	2:B:348:ILE:HD13	2.03	0.57
2:B:353:ASN:ND2	2:B:393:ILE:HA	2.20	0.57
2:D:354:LEU:HD21	2:D:399:PHE:CE1	2.40	0.57
2:B:390:ASN:CB	3:B:87:HOH:O	2.52	0.57
2:B:401:LYS:O	2:B:405:THR:CG2	2.54	0.56
2:B:356:GLU:HA	2:B:356:GLU:OE2	2.04	0.56
2:B:353:ASN:HD21	2:B:393:ILE:HD12	1.70	0.56
2:D:356:GLU:OE2	2:D:356:GLU:CA	2.54	0.56
2:D:341:LYS:CE	3:D:90:HOH:O	2.54	0.55
2:B:385:LEU:C	2:B:387:VAL:N	2.56	0.55
1:C:222:ARG:NH1	1:C:222:ARG:CG	2.65	0.55
1:A:186:GLU:CG	1:C:153:LYS:HD2	2.37	0.55
2:B:376:ASN:O	2:B:380:GLN:HG3	2.06	0.55
1:A:21:GLU:OE2	1:A:25:ARG:NH1	2.38	0.55
1:A:48:CYS:O	1:A:85:PBF:HD1	2.07	0.54
1:C:85:PBF:CI2	2:D:356:GLU:CD	2.74	0.54
1:A:143:MET:CE	1:A:165:THR:HA	2.37	0.54
2:B:401:LYS:O	2:B:405:THR:HG23	2.08	0.54
2:D:343:LEU:C	2:D:343:LEU:HD13	2.28	0.54
2:D:385:LEU:HG	2:D:385:LEU:O	2.08	0.53
2:D:343:LEU:HD13	2:D:343:LEU:O	2.09	0.53
2:D:353:ASN:HD22	2:D:393:ILE:HA	1.73	0.53
1:A:201:GLU:OE1	1:A:205:GLU:OE2	2.27	0.52
1:A:11:CYS:HB3	1:A:46:TRP:CD1	2.45	0.52
2:B:390:ASN:ND2	3:B:87:HOH:O	2.39	0.52
1:C:57:GLU:O	1:C:61:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:368:ASP:OD2	2:B:403:TYR:OH	2.16	0.52
1:A:186:GLU:CD	1:A:186:GLU:H	2.11	0.52
2:D:336:MET:HE3	2:D:370:ILE:O	2.10	0.52
2:D:355:SER:CA	2:D:393:ILE:HD11	2.40	0.51
2:B:376:ASN:C	2:B:380:GLN:NE2	2.64	0.50
2:B:386:ALA:O	2:B:390:ASN:HA	2.11	0.50
2:B:353:ASN:HD21	2:B:393:ILE:CG1	2.24	0.50
2:B:392:TYR:CE1	2:B:393:ILE:HG22	2.45	0.50
1:A:171:GLU:C	1:A:203:LYS:HG2	2.31	0.50
2:D:376:ASN:O	2:D:380:GLN:HG3	2.12	0.50
2:B:340:GLN:HE21	2:B:340:GLN:HA	1.77	0.49
2:D:337:ASP:C	2:D:337:ASP:OD1	2.49	0.49
1:A:3:GLY:HA2	2:B:392:TYR:CZ	2.48	0.49
2:B:353:ASN:ND2	2:B:393:ILE:HG13	2.28	0.48
1:C:58:PHE:HA	1:C:61:GLN:HE21	1.78	0.48
2:D:348:ILE:HD13	2:D:376:ASN:HA	1.96	0.48
1:C:53:THR:O	1:C:57:GLU:HG3	2.13	0.48
2:B:353:ASN:ND2	2:B:393:ILE:CG1	2.76	0.48
1:A:227:GLU:O	1:A:230:SER:O	2.31	0.47
2:B:378:ILE:HD13	2:B:403:TYR:CD1	2.48	0.47
2:D:405:THR:HG22	2:D:406:VAL:N	2.29	0.47
2:B:348:ILE:HD12	2:B:379:CYS:HB3	1.96	0.47
1:C:189:LYS:HD3	1:C:219:ILE:HG21	1.97	0.47
2:B:401:LYS:HA	2:B:401:LYS:HD3	1.59	0.46
1:C:58:PHE:HA	1:C:61:GLN:HG3	1.97	0.46
2:B:387:VAL:O	2:B:390:ASN:HB2	2.15	0.46
1:C:85:PBF:CI1	1:C:85:PBF:CE2	2.90	0.46
1:A:141:THR:H	1:A:144:HIS:HD2	1.60	0.46
2:D:371:SER:OG	2:D:373:ALA:HB3	2.15	0.46
2:D:384:MET:C	2:D:386:ALA:H	2.18	0.45
1:A:9:MET:HG2	3:A:315:HOH:O	2.16	0.45
1:A:143:MET:CE	1:A:175:PRO:CG	2.82	0.45
1:A:85:PBF:O	1:A:89:VAL:HG23	2.17	0.45
1:C:11:CYS:HB3	1:C:46:TRP:CD1	2.51	0.45
2:B:349:THR:HA	2:B:352:MET:HG3	1.99	0.45
2:D:367:PRO:HG2	2:D:367:PRO:O	2.16	0.45
2:B:401:LYS:O	2:B:402:ALA:C	2.55	0.45
1:C:85:PBF:HI1	1:C:85:PBF:CE2	2.45	0.45
2:D:384:MET:HA	2:D:387:VAL:HG12	1.99	0.45
1:A:221:LYS:C	1:A:221:LYS:HD3	2.36	0.45
1:A:5:VAL:O	2:B:391:ARG:HD3	2.16	0.45
1:A:143:MET:HE3	1:A:165:THR:HA	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:353:ASN:HD21	2:B:393:ILE:CD1	2.30	0.45
2:B:385:LEU:O	2:B:386:ALA:C	2.55	0.44
1:A:23:LYS:HG2	1:A:58:PHE:CE1	2.53	0.44
1:A:85:PBF:CI2	2:B:356:GLU:CD	2.83	0.44
1:C:141:THR:OG1	1:C:144:HIS:CD2	2.66	0.44
1:C:135:LYS:HE2	1:C:139:ASP:OD1	2.18	0.44
1:C:219:ILE:N	1:C:219:ILE:HD13	2.31	0.43
2:D:354:LEU:HD21	2:D:399:PHE:CZ	2.53	0.43
1:C:152:LEU:HD22	1:C:156:HIS:CD2	2.52	0.43
2:D:390:ASN:HB2	2:D:392:TYR:CE2	2.53	0.43
2:D:376:ASN:C	2:D:380:GLN:HE21	2.22	0.43
2:B:375:ILE:O	2:B:376:ASN:C	2.55	0.43
2:D:348:ILE:C	2:D:350:SER:N	2.71	0.43
2:B:402:ALA:O	2:B:405:THR:HG23	2.19	0.42
2:D:374:ASP:O	2:D:377:SER:HB2	2.19	0.42
2:D:349:THR:HG21	2:D:360:LEU:HD11	2.01	0.42
2:D:400:GLU:O	2:D:404:LYS:CD	2.64	0.42
2:B:405:THR:OG1	2:B:406:VAL:N	2.53	0.42
2:B:386:ALA:HB1	2:B:391:ARG:O	2.20	0.42
2:D:376:ASN:C	2:D:380:GLN:NE2	2.72	0.42
2:B:388:ARG:HA	2:B:388:ARG:HD3	1.80	0.41
2:D:403:TYR:O	2:D:407:ILE:HB	2.21	0.41
2:B:392:TYR:N	2:B:392:TYR:HD1	2.12	0.41
2:B:387:VAL:CG1	2:B:390:ASN:OD1	2.63	0.41
2:D:378:ILE:HD11	2:D:407:ILE:CD1	2.47	0.41
2:D:343:LEU:HD22	2:D:343:LEU:HA	1.79	0.41
2:D:336:MET:HG3	2:D:337:ASP:N	2.35	0.41
1:A:85:PBF:CE2	1:A:85:PBF:CI1	2.98	0.41
2:D:375:ILE:O	2:D:376:ASN:C	2.59	0.40
1:A:19:LEU:HD13	1:A:55:ILE:HG12	2.04	0.40
2:B:397:LYS:HB2	2:B:397:LYS:HE2	1.92	0.40
2:B:401:LYS:O	2:B:405:THR:HG22	2.22	0.40
2:B:376:ASN:CB	2:B:380:GLN:HE21	2.35	0.40

All (1) 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	Distance(Å)	Clash(Å)
3:C:312:HOH:O	3:C:369:HOH:O[8_654]	2.07	0.13

## 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	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
1	C	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
2	B	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
2	D	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
All	All	594/628 (95%)	580 (98%)	14 (2%)	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	181/183 (99%)	171 (94%)	10 (6%)	30	20
1	C	181/183 (99%)	170 (94%)	11 (6%)	26	16
2	B	66/76 (87%)	51 (77%)	15 (23%)	1	0
2	D	66/76 (87%)	59 (89%)	7 (11%)	10	3
All	All	494/518 (95%)	451 (91%)	43 (9%)	15	7

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	95	LYS
1	A	104	GLN
1	A	152	LEU
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	216	LEU
1	A	221	LYS
1	A	222	ARG
1	A	230	SER
2	B	340	GLN
2	B	343	LEU
2	B	348	ILE
2	B	351	LYS
2	B	356	GLU
2	B	367	PRO
2	B	369	LYS
2	B	384	MET
2	B	387	VAL
2	B	388	ARG
2	B	391	ARG
2	B	392	TYR
2	B	397	LYS
2	B	401	LYS
2	B	405	THR
1	C	10	ILE
1	C	25	ARG
1	C	35	ARG
1	C	61	GLN
1	C	95	LYS
1	C	152	LEU
1	C	178	LEU
1	C	209	LEU
1	C	216	LEU
1	C	218	LEU
1	C	219	ILE
2	D	337	ASP
2	D	340	GLN
2	D	356	GLU
2	D	367	PRO
2	D	391	ARG
2	D	393	ILE
2	D	397	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	38	GLN
1	A	104	GLN
1	A	144	HIS
2	B	340	GLN
2	B	353	ASN
2	B	380	GLN
1	C	38	GLN
1	C	61	GLN
1	C	144	HIS
1	C	194	GLN
2	D	340	GLN
2	D	353	ASN
2	D	380	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	$\# Z  > 2$
1	PBF	A	85	1,2	19,19,21	4.73	5 (26%)	21,24,28	5.35	7 (33%)
1	PBF	C	85	1,2	19,19,21	4.54	5 (26%)	21,24,28	3.22	5 (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
1	PBF	A	85	1,2	-	0/8/10/16	0/2/2/2
1	PBF	C	85	1,2	-	0/8/10/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	PBF	O-C	17.36	1.23	1.11
1	A	85	PBF	O-C	17.01	1.23	1.11
1	A	85	PBF	CB-CG	9.34	1.74	1.51
1	C	85	PBF	CB-CG	-6.64	1.34	1.51
1	A	85	PBF	CN1-CZ	-4.85	1.45	1.56
1	C	85	PBF	CB-CA	3.70	1.63	1.53
1	A	85	PBF	CB-CA	3.43	1.62	1.53
1	A	85	PBF	CN1-CT	-2.75	1.50	1.56
1	C	85	PBF	CN1-CZ	-2.43	1.51	1.56
1	C	85	PBF	CN1-CT	-2.06	1.52	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	PBF	CG-CB-CA	15.21	150.32	114.42
1	A	85	PBF	C-CA-N	-12.91	100.93	113.83
1	C	85	PBF	CG-CB-CA	11.55	141.68	114.42
1	A	85	PBF	CB-CG-CD2	-9.50	102.26	120.90
1	A	85	PBF	CB-CG-CD1	6.66	133.98	120.90
1	A	85	PBF	CB-CA-N	-6.13	83.48	112.03
1	C	85	PBF	CB-CA-N	-5.58	86.05	112.03
1	C	85	PBF	C-CA-N	-4.03	109.81	113.83
1	C	85	PBF	CB-CG-CD2	-3.80	113.44	120.90
1	A	85	PBF	CD2-CG-CD1	3.03	123.26	118.16
1	A	85	PBF	CE1-CD1-CG	-2.45	117.44	121.05
1	C	85	PBF	CD2-CG-CD1	2.11	121.71	118.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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	229/231 (99%)	-0.49	2 (0%) 81 83	20, 28, 48, 104	0
1	C	229/231 (99%)	-0.54	2 (0%) 81 83	20, 27, 48, 104	0
2	B	73/83 (87%)	0.15	3 (4%) 35 34	28, 52, 81, 91	0
2	D	73/83 (87%)	0.30	5 (6%) 17 15	29, 52, 84, 101	0
All	All	604/628 (96%)	-0.34	12 (1%) 62 63	20, 30, 69, 104	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	MET	4.8
1	C	231	MET	4.3
2	D	387	VAL	3.0
2	D	389	GLU	3.0
2	B	392	TYR	2.9
2	B	354	LEU	2.5
2	D	392	TYR	2.5
1	C	3	GLY	2.4
2	D	406	VAL	2.3
2	B	382	SER	2.3
2	D	336	MET	2.2
1	A	3	GLY	2.1

### 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. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PBF	C	85	18/20	0.14	1.49	19,45,70,78	0
1	PBF	A	85	18/20	0.15	1.25	21,39,73,76	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.