Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:13 pm BST

PDB ID	:	5MSK
Title	:	Mouse PA28beta
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2017-01-05
Resolution	:	3.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

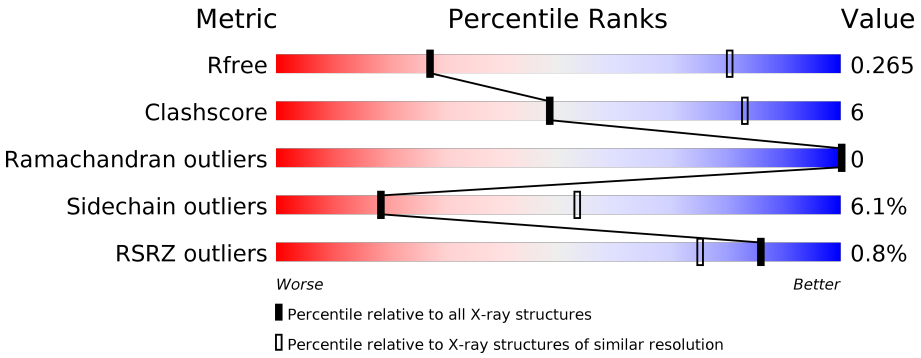
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	70% 15% • 12%
1	B	239	69% 15% • 12%
1	C	239	% 67% 15% • 14%
1	D	239	% 69% 14% • 13%
1	E	239	% 68% 14% • 16%
1	F	239	71% 14% • 13%

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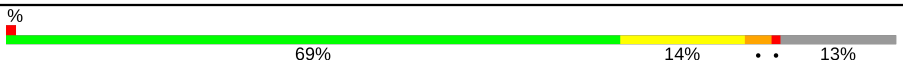
Mol	Chain	Length	Quality of chain
1	G	239	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11546 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 activator complex subunit 2.

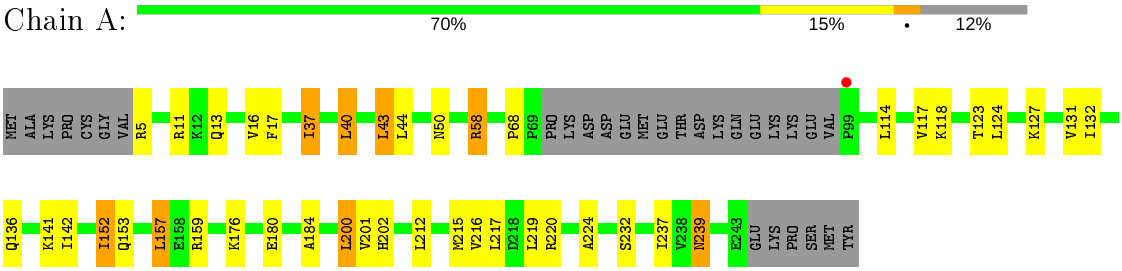
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1670	1072	284	309	5			
1	B	211	Total	C	N	O	S	0	0	0
			1676	1074	285	312	5			
1	C	206	Total	C	N	O	S	0	0	0
			1645	1056	278	306	5			
1	D	207	Total	C	N	O	S	0	0	0
			1645	1056	280	304	5			
1	E	201	Total	C	N	O	S	0	0	0
			1602	1031	271	295	5			
1	F	208	Total	C	N	O	S	0	0	0
			1654	1061	281	307	5			
1	G	208	Total	C	N	O	S	0	0	0
			1654	1061	281	307	5			

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 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.

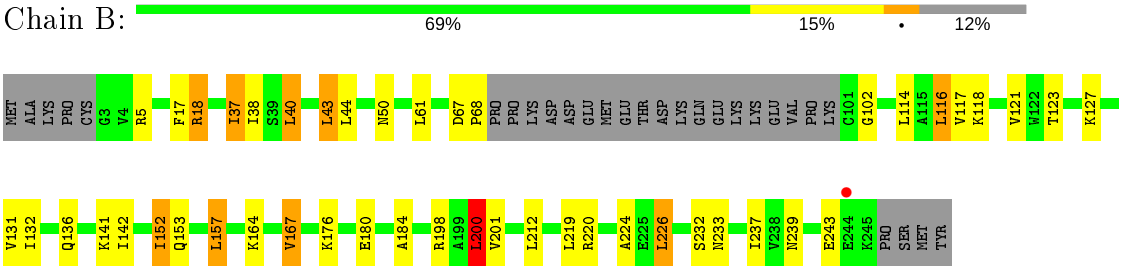
- Molecule 1: Proteasome activator complex subunit 2

Chain A:



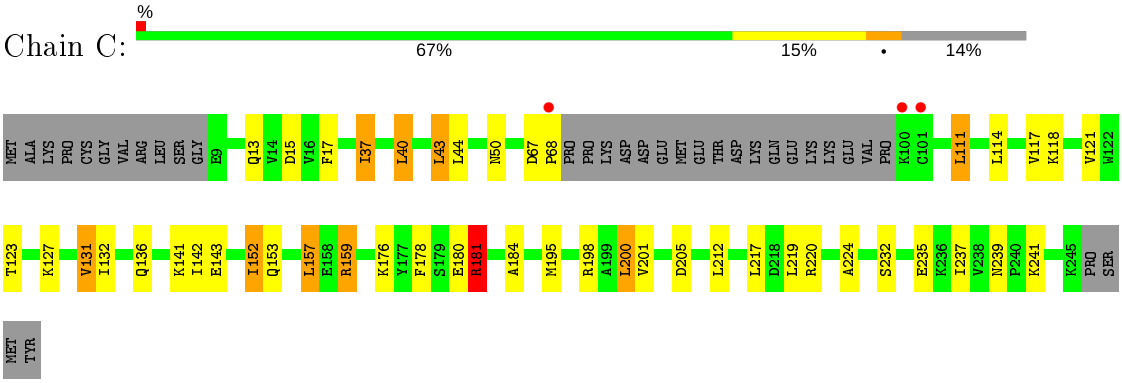
- Molecule 1: Proteasome activator complex subunit 2

Chain B:



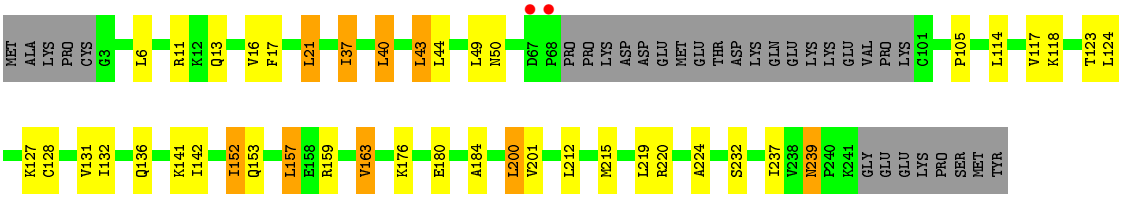
- Molecule 1: Proteasome activator complex subunit 2

Chain C:

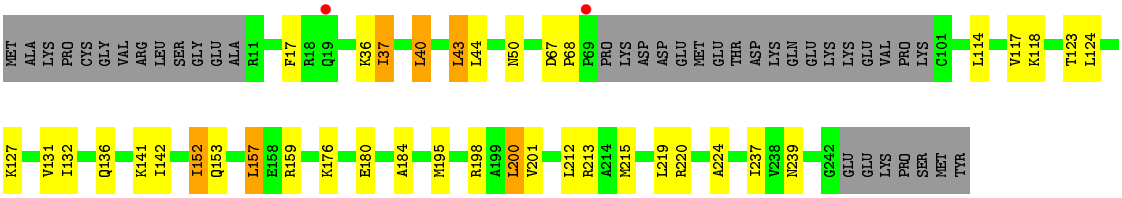


- Molecule 1: Proteasome activator complex subunit 2

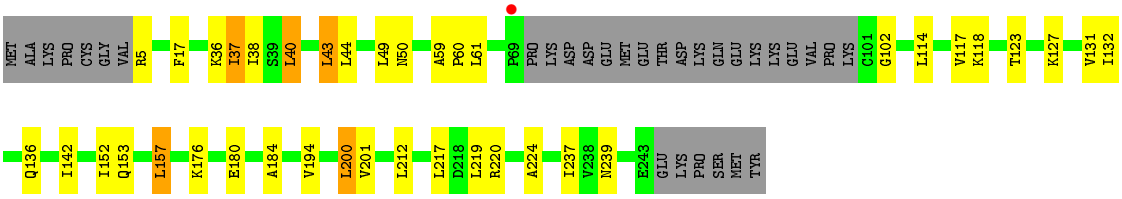
Chain D:



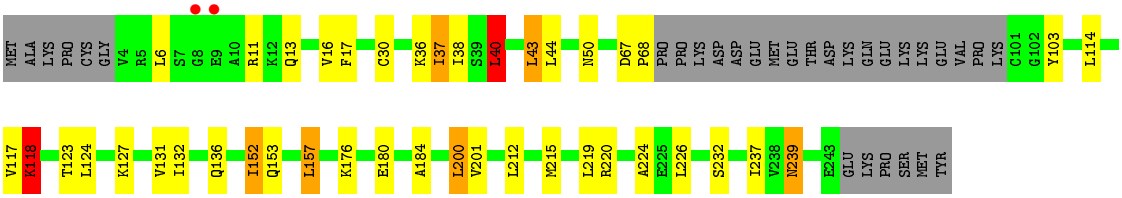
• Molecule 1: Proteasome activator complex subunit 2



• Molecule 1: Proteasome activator complex subunit 2



• Molecule 1: Proteasome activator complex subunit 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.84Å 132.61Å 90.93Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-3.60) 97.8 (30.00-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.56Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.242 , 0.263 0.242 , 0.265	Depositor DCC
R_{free} test set	1170 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	108.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.028 for h,-k,-l 0.013 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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	0.46	1/1701 (0.1%)	1.04	8/2302 (0.3%)
1	B	0.47	3/1705 (0.2%)	1.15	14/2306 (0.6%)
1	C	0.48	1/1674 (0.1%)	1.22	14/2264 (0.6%)
1	D	0.49	2/1674 (0.1%)	0.80	8/2266 (0.4%)
1	E	0.42	1/1632 (0.1%)	0.92	7/2211 (0.3%)
1	F	0.41	0/1684	0.77	4/2280 (0.2%)
1	G	0.42	1/1683 (0.1%)	0.80	5/2278 (0.2%)
All	All	0.45	9/11753 (0.1%)	0.97	60/15907 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	VAL	CB-CG2	10.10	1.74	1.52
1	A	159	ARG	CZ-NH1	9.38	1.45	1.33
1	C	15	ASP	CG-OD2	7.10	1.41	1.25
1	B	18	ARG	CZ-NH2	6.61	1.41	1.33
1	G	118	LYS	CD-CE	6.53	1.67	1.51
1	D	159	ARG	CZ-NH1	6.02	1.40	1.33
1	B	167	VAL	CB-CG1	5.83	1.65	1.52
1	E	213	ARG	CZ-NH1	5.57	1.40	1.33
1	B	167	VAL	CB-CG2	5.42	1.64	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	131	VAL	CG1-CB-CG2	-30.78	61.65	110.90
1	B	18	ARG	NE-CZ-NH1	-25.80	107.40	120.30
1	A	58	ARG	NE-CZ-NH1	-22.09	109.25	120.30
1	A	58	ARG	NE-CZ-NH2	20.95	130.78	120.30
1	B	18	ARG	NE-CZ-NH2	20.56	130.58	120.30
1	C	181	ARG	NE-CZ-NH1	-19.52	110.54	120.30
1	C	181	ARG	NE-CZ-NH2	19.45	130.03	120.30
1	E	159	ARG	NE-CZ-NH1	-17.00	111.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	159	ARG	NE-CZ-NH2	16.62	128.61	120.30
1	B	167	VAL	CG1-CB-CG2	-13.91	88.65	110.90
1	G	40	LEU	CA-CB-CG	11.65	142.10	115.30
1	A	40	LEU	CA-CB-CG	11.56	141.89	115.30
1	B	40	LEU	CA-CB-CG	11.45	141.64	115.30
1	A	58	ARG	CD-NE-CZ	10.53	138.35	123.60
1	C	181	ARG	CD-NE-CZ	9.88	137.43	123.60
1	B	18	ARG	CD-NE-CZ	9.15	136.41	123.60
1	B	18	ARG	CG-CD-NE	-8.39	94.18	111.80
1	B	200	LEU	CA-CB-CG	7.94	133.57	115.30
1	B	167	VAL	CB-CA-C	7.76	126.15	111.40
1	E	159	ARG	CD-NE-CZ	7.15	133.61	123.60
1	C	159	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	C	15	ASP	CB-CG-OD2	6.82	124.43	118.30
1	C	43	LEU	CA-CB-CG	6.72	130.76	115.30
1	G	43	LEU	CA-CB-CG	6.72	130.76	115.30
1	D	21	LEU	CB-CG-CD2	6.68	122.35	111.00
1	A	43	LEU	CA-CB-CG	6.66	130.63	115.30
1	B	43	LEU	CA-CB-CG	6.66	130.62	115.30
1	E	43	LEU	CA-CB-CG	6.66	130.62	115.30
1	F	43	LEU	CA-CB-CG	6.60	130.47	115.30
1	D	21	LEU	CA-CB-CG	6.56	130.39	115.30
1	C	159	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	163	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	C	159	ARG	CG-CD-NE	6.17	124.75	111.80
1	B	200	LEU	CB-CG-CD2	6.03	121.26	111.00
1	G	40	LEU	CB-CG-CD1	6.02	121.23	111.00
1	F	40	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	40	LEU	CA-CB-CG	5.91	128.89	115.30
1	C	40	LEU	CA-CB-CG	5.89	128.84	115.30
1	E	40	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	43	LEU	CB-CG-CD1	5.86	120.96	111.00
1	B	40	LEU	CB-CG-CD1	5.67	120.64	111.00
1	G	200	LEU	CA-CB-CG	5.66	128.33	115.30
1	C	200	LEU	CA-CB-CG	5.63	128.25	115.30
1	F	200	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	40	LEU	CB-CG-CD1	5.57	120.47	111.00
1	D	200	LEU	CA-CB-CG	5.54	128.04	115.30
1	E	200	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	200	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	116	LEU	CB-CG-CD1	5.36	120.11	111.00
1	C	159	ARG	CB-CG-CD	5.33	125.45	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	111	LEU	CA-CB-CG	-5.30	103.10	115.30
1	A	131	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	D	131	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	E	131	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	G	131	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	B	131	VAL	CG1-CB-CG2	-5.25	102.51	110.90
1	D	163	VAL	N-CA-CB	5.24	123.03	111.50
1	B	226	LEU	CB-CG-CD1	5.20	119.85	111.00
1	F	131	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	C	131	VAL	CB-CA-C	-5.08	101.75	111.40

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	1670	0	1710	25	0
1	B	1676	0	1713	27	0
1	C	1645	0	1682	26	0
1	D	1645	0	1685	24	0
1	E	1602	0	1640	21	0
1	F	1654	0	1689	20	0
1	G	1654	0	1691	24	0
All	All	11546	0	11810	140	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 (140) 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:F:59:ALA:HB1	1:F:60:PRO:HD2	1.64	0.79
1:A:136:GLN:HG2	1:A:157:LEU:HD11	1.69	0.74
1:B:136:GLN:HG2	1:B:157:LEU:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:GLN:HG2	1:D:157:LEU:HD11	1.70	0.73
1:E:136:GLN:HG2	1:E:157:LEU:HD11	1.70	0.73
1:G:136:GLN:HG2	1:G:157:LEU:HD11	1.70	0.73
1:F:136:GLN:HG2	1:F:157:LEU:HD11	1.71	0.73
1:C:136:GLN:HG2	1:C:157:LEU:HD11	1.69	0.73
1:F:59:ALA:HB1	1:F:60:PRO:CD	2.19	0.72
1:F:37:ILE:HD11	1:F:224:ALA:HA	1.75	0.69
1:B:37:ILE:HD11	1:B:224:ALA:HA	1.74	0.69
1:G:37:ILE:HD11	1:G:224:ALA:HA	1.74	0.69
1:C:37:ILE:HD11	1:C:224:ALA:HA	1.75	0.68
1:D:37:ILE:HD11	1:D:224:ALA:HA	1.74	0.68
1:E:37:ILE:HD11	1:E:224:ALA:HA	1.75	0.67
1:A:37:ILE:HD11	1:A:224:ALA:HA	1.75	0.67
1:A:5:ARG:N	1:G:30:CYS:HG	1.97	0.62
1:D:152:ILE:HD11	1:E:142:ILE:HB	1.82	0.62
1:G:6:LEU:HB2	1:G:11:ARG:HG2	1.82	0.61
1:G:13:GLN:HA	1:G:16:VAL:HG22	1.83	0.60
1:C:152:ILE:HD11	1:D:142:ILE:HB	1.84	0.60
1:F:44:LEU:O	1:F:50:ASN:ND2	2.35	0.60
1:G:44:LEU:O	1:G:50:ASN:ND2	2.35	0.60
1:B:200:LEU:HB2	1:C:178:PHE:HB3	1.84	0.59
1:A:13:GLN:HA	1:A:16:VAL:HG22	1.85	0.59
1:B:152:ILE:HD11	1:C:142:ILE:HB	1.83	0.59
1:D:44:LEU:O	1:D:50:ASN:ND2	2.36	0.59
1:E:44:LEU:O	1:E:50:ASN:ND2	2.34	0.59
1:A:44:LEU:O	1:A:50:ASN:ND2	2.36	0.58
1:C:181:ARG:HD2	1:C:205:ASP:OD1	2.03	0.58
1:A:117:VAL:HG21	1:A:212:LEU:HD22	1.86	0.58
1:F:117:VAL:HG21	1:F:212:LEU:HD22	1.86	0.58
1:E:117:VAL:HG21	1:E:212:LEU:HD22	1.86	0.57
1:C:117:VAL:HG21	1:C:212:LEU:HD22	1.86	0.57
1:G:117:VAL:HG21	1:G:212:LEU:HD22	1.86	0.57
1:C:44:LEU:O	1:C:50:ASN:ND2	2.36	0.57
1:B:117:VAL:HG21	1:B:212:LEU:HD22	1.87	0.56
1:A:152:ILE:HD11	1:B:142:ILE:HB	1.87	0.56
1:B:44:LEU:O	1:B:50:ASN:ND2	2.36	0.56
1:E:195:MET:HG3	1:E:198:ARG:HD2	1.88	0.56
1:D:117:VAL:HG21	1:D:212:LEU:HD22	1.86	0.56
1:B:233:ASN:OD1	1:C:141:LYS:HA	2.07	0.55
1:G:114:LEU:O	1:G:118:LYS:HB2	2.08	0.54
1:B:232:SER:O	1:C:141:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:THR:O	1:C:127:LYS:HG2	2.08	0.54
1:B:220:ARG:HD3	1:C:17:PHE:CE1	2.42	0.54
1:B:114:LEU:O	1:B:118:LYS:HB2	2.08	0.54
1:C:114:LEU:O	1:C:118:LYS:HB2	2.08	0.54
1:E:114:LEU:O	1:E:118:LYS:HB2	2.08	0.54
1:B:123:THR:O	1:B:127:LYS:HG2	2.07	0.54
1:G:123:THR:O	1:G:127:LYS:HG2	2.08	0.54
1:A:123:THR:O	1:A:127:LYS:HG2	2.09	0.53
1:A:114:LEU:O	1:A:118:LYS:HB2	2.08	0.53
1:F:59:ALA:CB	1:F:60:PRO:CD	2.85	0.53
1:B:61:LEU:HD23	1:B:198:ARG:HE	1.73	0.53
1:D:123:THR:O	1:D:127:LYS:HG2	2.08	0.53
1:E:123:THR:O	1:E:127:LYS:HG2	2.09	0.53
1:B:121:VAL:HG13	1:B:167:VAL:HG23	1.90	0.53
1:F:114:LEU:O	1:F:118:LYS:HB2	2.08	0.53
1:F:153:GLN:NE2	1:F:237:ILE:O	2.42	0.53
1:A:142:ILE:HB	1:G:152:ILE:HD11	1.89	0.53
1:D:114:LEU:O	1:D:118:LYS:HB2	2.08	0.53
1:B:153:GLN:NE2	1:B:237:ILE:O	2.43	0.52
1:F:123:THR:O	1:F:127:LYS:HG2	2.09	0.52
1:A:17:PHE:CE1	1:G:220:ARG:HD3	2.45	0.52
1:A:153:GLN:NE2	1:A:237:ILE:O	2.43	0.52
1:C:153:GLN:NE2	1:C:237:ILE:O	2.43	0.52
1:A:13:GLN:O	1:G:38:ILE:HD11	2.10	0.51
1:G:153:GLN:NE2	1:G:237:ILE:O	2.43	0.51
1:D:132:ILE:O	1:D:136:GLN:HG3	2.11	0.51
1:E:153:GLN:NE2	1:E:237:ILE:O	2.43	0.51
1:C:132:ILE:O	1:C:136:GLN:HG3	2.11	0.51
1:B:132:ILE:O	1:B:136:GLN:HG3	2.11	0.51
1:D:153:GLN:NE2	1:D:237:ILE:O	2.43	0.51
1:C:220:ARG:HD3	1:D:17:PHE:CE1	2.46	0.51
1:A:220:ARG:HD3	1:B:17:PHE:CE1	2.47	0.50
1:C:232:SER:O	1:D:141:LYS:HG3	2.11	0.50
1:E:132:ILE:O	1:E:136:GLN:HG3	2.12	0.50
1:E:220:ARG:HD3	1:F:17:PHE:CE1	2.46	0.50
1:D:232:SER:O	1:E:141:LYS:HG3	2.12	0.49
1:G:132:ILE:O	1:G:136:GLN:HG3	2.12	0.49
1:F:132:ILE:O	1:F:136:GLN:HG3	2.12	0.49
1:B:176:LYS:O	1:B:180:GLU:HB2	2.13	0.49
1:D:6:LEU:HD13	1:D:11:ARG:HG3	1.95	0.49
1:A:176:LYS:O	1:A:180:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:O	1:A:136:GLN:HG3	2.12	0.48
1:G:176:LYS:O	1:G:180:GLU:HB2	2.13	0.48
1:F:176:LYS:O	1:F:180:GLU:HB2	2.13	0.48
1:C:176:LYS:O	1:C:180:GLU:HB2	2.14	0.48
1:D:176:LYS:O	1:D:180:GLU:HB2	2.14	0.47
1:E:176:LYS:O	1:E:180:GLU:HB2	2.14	0.47
1:A:141:LYS:HG3	1:G:232:SER:O	2.15	0.47
1:D:128:CYS:SG	1:D:163:VAL:HG23	2.54	0.47
1:B:164:LYS:HA	1:B:167:VAL:HG12	1.97	0.46
1:F:59:ALA:CB	1:F:60:PRO:HD2	2.40	0.45
1:A:232:SER:O	1:B:141:LYS:HG3	2.16	0.45
1:D:220:ARG:HD3	1:E:17:PHE:CE1	2.52	0.45
1:E:67:ASP:HA	1:E:68:PRO:HD3	1.88	0.44
1:G:215:MET:O	1:G:219:LEU:HG	2.18	0.44
1:F:38:ILE:HD11	1:G:13:GLN:O	2.16	0.44
1:G:124:LEU:HD23	1:G:219:LEU:HD22	1.99	0.44
1:D:124:LEU:HD23	1:D:219:LEU:HD22	1.99	0.44
1:A:124:LEU:HD23	1:A:219:LEU:HD22	1.99	0.44
1:F:220:ARG:HD3	1:G:17:PHE:CE1	2.53	0.44
1:E:124:LEU:HD23	1:E:219:LEU:HD22	2.00	0.44
1:E:68:PRO:HG3	1:F:102:GLY:HA3	1.99	0.43
1:A:68:PRO:HG3	1:B:102:GLY:HA2	2.00	0.43
1:G:36:LYS:O	1:G:40:LEU:HD13	2.19	0.43
1:B:121:VAL:CG1	1:B:167:VAL:HG23	2.48	0.43
1:E:184:ALA:HB1	1:E:201:VAL:HG22	2.01	0.43
1:E:215:MET:O	1:E:219:LEU:HG	2.19	0.42
1:C:143:GLU:OE1	1:C:241:LYS:NZ	2.41	0.42
1:D:215:MET:O	1:D:219:LEU:HG	2.19	0.42
1:G:67:ASP:HA	1:G:68:PRO:HD3	1.88	0.42
1:A:215:MET:O	1:A:219:LEU:HG	2.20	0.42
1:F:184:ALA:HB1	1:F:201:VAL:HG22	2.02	0.42
1:E:152:ILE:HD11	1:F:142:ILE:HB	2.02	0.42
1:G:184:ALA:HB1	1:G:201:VAL:HG22	2.01	0.42
1:B:184:ALA:HB1	1:B:201:VAL:HG22	2.01	0.42
1:C:195:MET:HG3	1:D:105:PRO:HA	2.02	0.42
1:D:13:GLN:HA	1:D:16:VAL:HG22	2.01	0.41
1:C:235:GLU:OE1	1:C:235:GLU:HA	2.20	0.41
1:C:184:ALA:HB1	1:C:201:VAL:HG22	2.02	0.41
1:D:184:ALA:HB1	1:D:201:VAL:HG22	2.02	0.41
1:A:58:ARG:HG3	1:A:202:HIS:CD2	2.55	0.41
1:C:132:ILE:HG23	1:C:136:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HA	1:B:68:PRO:HD3	1.87	0.41
1:A:184:ALA:HB1	1:A:201:VAL:HG22	2.02	0.41
1:D:132:ILE:HG23	1:D:136:GLN:HE21	1.86	0.41
1:E:132:ILE:HG23	1:E:136:GLN:HE21	1.86	0.41
1:C:117:VAL:O	1:C:121:VAL:HG23	2.21	0.41
1:A:132:ILE:HG23	1:A:136:GLN:HE21	1.85	0.41
1:A:239:ASN:O	1:A:239:ASN:ND2	2.53	0.41
1:B:38:ILE:HD11	1:C:13:GLN:O	2.20	0.40
1:D:239:ASN:O	1:D:239:ASN:ND2	2.54	0.40
1:B:132:ILE:HG23	1:B:136:GLN:HE21	1.87	0.40
1:B:117:VAL:O	1:B:121:VAL:HG23	2.22	0.40
1:C:67:ASP:HA	1:C:68:PRO:HD3	1.88	0.40
1:F:61:LEU:HD12	1:F:61:LEU:HA	1.80	0.40
1:G:239:ASN:O	1:G:239:ASN:ND2	2.54	0.40

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	206/239 (86%)	199 (97%)	7 (3%)	0	100	100
1	B	207/239 (87%)	200 (97%)	7 (3%)	0	100	100
1	C	202/239 (84%)	195 (96%)	7 (4%)	0	100	100
1	D	203/239 (85%)	196 (97%)	7 (3%)	0	100	100
1	E	197/239 (82%)	190 (96%)	7 (4%)	0	100	100
1	F	204/239 (85%)	198 (97%)	6 (3%)	0	100	100
1	G	204/239 (85%)	196 (96%)	8 (4%)	0	100	100
All	All	1423/1673 (85%)	1374 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	183/210 (87%)	173 (94%)	10 (6%)	21 57
1	B	183/210 (87%)	170 (93%)	13 (7%)	14 48
1	C	180/210 (86%)	166 (92%)	14 (8%)	12 44
1	D	180/210 (86%)	171 (95%)	9 (5%)	24 59
1	E	176/210 (84%)	168 (96%)	8 (4%)	27 62
1	F	181/210 (86%)	168 (93%)	13 (7%)	14 47
1	G	181/210 (86%)	171 (94%)	10 (6%)	21 57
All	All	1264/1470 (86%)	1187 (94%)	77 (6%)	18 53

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	37	ILE
1	A	40	LEU
1	A	43	LEU
1	A	152	ILE
1	A	157	LEU
1	A	200	LEU
1	A	216	VAL
1	A	217	LEU
1	A	239	ASN
1	B	5	ARG
1	B	18	ARG
1	B	37	ILE
1	B	40	LEU
1	B	43	LEU
1	B	116	LEU
1	B	152	ILE
1	B	157	LEU
1	B	200	LEU
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	226	LEU
1	B	239	ASN
1	B	243	GLU
1	C	37	ILE
1	C	40	LEU
1	C	43	LEU
1	C	111	LEU
1	C	131	VAL
1	C	152	ILE
1	C	157	LEU
1	C	159	ARG
1	C	181	ARG
1	C	198	ARG
1	C	200	LEU
1	C	217	LEU
1	C	219	LEU
1	C	239	ASN
1	D	21	LEU
1	D	37	ILE
1	D	40	LEU
1	D	43	LEU
1	D	49	LEU
1	D	152	ILE
1	D	157	LEU
1	D	200	LEU
1	D	239	ASN
1	E	36	LYS
1	E	37	ILE
1	E	40	LEU
1	E	43	LEU
1	E	152	ILE
1	E	157	LEU
1	E	200	LEU
1	E	239	ASN
1	F	5	ARG
1	F	36	LYS
1	F	37	ILE
1	F	40	LEU
1	F	43	LEU
1	F	49	LEU
1	F	152	ILE
1	F	157	LEU

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Mol	Chain	Res	Type
1	F	194	VAL
1	F	200	LEU
1	F	217	LEU
1	F	219	LEU
1	F	239	ASN
1	G	37	ILE
1	G	40	LEU
1	G	43	LEU
1	G	103	TYR
1	G	118	LYS
1	G	152	ILE
1	G	157	LEU
1	G	200	LEU
1	G	226	LEU
1	G	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	B	136	GLN
1	C	136	GLN
1	D	13	GLN
1	D	136	GLN
1	E	136	GLN
1	F	136	GLN
1	G	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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^{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	210/239 (87%)	-0.28	1 (0%)	91	83	78, 103, 148, 173	0
1	B	211/239 (88%)	-0.31	1 (0%)	91	83	71, 100, 141, 160	0
1	C	206/239 (86%)	-0.30	3 (1%)	73	60	79, 109, 150, 176	0
1	D	207/239 (86%)	-0.33	2 (0%)	82	70	82, 110, 148, 175	0
1	E	201/239 (84%)	-0.28	2 (0%)	82	70	81, 106, 152, 189	0
1	F	208/239 (87%)	-0.32	1 (0%)	91	83	30, 113, 148, 184	0
1	G	208/239 (87%)	-0.23	2 (0%)	82	70	90, 115, 183, 221	0
All	All	1451/1673 (86%)	-0.29	12 (0%)	86	75	30, 109, 152, 221	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	GLU	3.1
1	A	99	PRO	2.9
1	G	8	GLY	2.9
1	E	69	PRO	2.7
1	B	244	GLU	2.6
1	D	68	PRO	2.5
1	F	69	PRO	2.5
1	C	101	CYS	2.3
1	E	19	GLN	2.3
1	C	68	PRO	2.3
1	C	100	LYS	2.2
1	D	67	ASP	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.