

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 03:08 AM EDT

PDB ID	:	7M5C
Title	:	Crystal Structure of human BAK in complex with WT BAK BH3 peptide
Authors	:	Singh, G.; Aggarwal, A.; Moldoveanu, T.
Deposited on	:	2021-03-23
Resolution	:	3.06 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 (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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.06 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.



Motria	Whole archive	Similar resolution		
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	1754 (3.10-3.02)		
Clashscore	141614	1864 (3.10-3.02)		
Ramachandran outliers	138981	1794 (3.10-3.02)		
Sidechain outliers	138945	1793 (3.10-3.02)		
RSRZ outliers	127900	1713 (3.10-3.02)		

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 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	А	166	78%	13%		9%
1	С	166	% 7 6%	15%		9%
1	Е	166	84%		11%	5%
1	G	166	.% 77%	7%	16%)
1	Ι	166	% 7 6%	11%	13'	%



Chain Length Quality of chain Mol Κ 1 16677% 12% 11% М 1661 76% 14% 10% .% 1 Ο 16681% 10% 9% 2% Q 1661 81% 7% 11% .% \mathbf{S} 1 16679% 7% 14% В 22568% 20% 12% 2D 2540% 28% 32% F 22584% 12% • 2Η 2576% 12% 12% J 22576% • 20% 2L 2564% 24% 12% 2Ν 2556% 20% 24% 2Р 2560% 12% 24% • 2R 2560% 16% 24% Т 22528% 56% 16%

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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13528 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	151	Total	С	Ν	0	S	0	0	0
1	A	101	1213	770	213	226	4	0	0	0
1	С	151	Total	С	Ν	0	S	0	0	0
1		101	1216	776	214	222	4	0	0	0
1	E	157	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	157	1260	802	221	232	5	0	0	0
1	C	130	Total	С	Ν	Ο	S	0	0	0
1	G	155	1123	717	200	203	3	0	0	
1	т	145	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	L	140	1159	740	203	212	4	0	0	0
1	K	147	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	11	141	1185	754	209	218	4	0		
1	М	1/0	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	111	145	1201	764	212	221	4	0	0	0
1	0	151	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	U	101	1209	770	213	221	5	0	0	0
1	1 0	147	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	<u>५</u>	1.71	1199	766	210	219	4	0	L	0
1	S	1/13	Total	С	Ν	0	S	0	0	0
	U U	140	1140	728	204	204	4	0	0	0

• Molecule 1 is a protein called Bcl-2 homologous antagonist/killer.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	166	SER	CYS	conflict	UNP Q16611
А	184	CYS	GLY	conflict	UNP Q16611
С	166	SER	CYS	conflict	UNP Q16611
С	184	CYS	GLY	conflict	UNP Q16611
Е	166	SER	CYS	conflict	UNP Q16611
Е	184	CYS	GLY	conflict	UNP Q16611
G	166	SER	CYS	conflict	UNP Q16611
G	184	CYS	GLY	conflict	UNP Q16611
Ι	166	SER	CYS	conflict	UNP Q16611



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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	184	CYS	GLY	conflict	UNP Q16611
K	166	SER	CYS	conflict	UNP Q16611
K	184	CYS	GLY	conflict	UNP Q16611
М	166	SER	CYS	conflict	UNP Q16611
М	184	CYS	GLY	conflict	UNP Q16611
0	166	SER	CYS	conflict	UNP Q16611
0	184	CYS	GLY	conflict	UNP Q16611
Q	166	SER	CYS	conflict	UNP Q16611
Q	184	CYS	GLY	conflict	UNP Q16611
S	166	SER	CYS	conflict	UNP Q16611
S	184	CYS	GLY	conflict	UNP Q16611

• Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	A	toms			ZeroOcc	AltConf	Trace
2	В	22	Total C	Ν	0	S	0	0	0
2	D		164 99	31	33	1	0	0	0
2	О	17	Total C	Ν	Ο	\mathbf{S}	0	0	0
		11	119 70	23	25	1	0	0	0
2	F	24	Total C	Ν	Ο	\mathbf{S}	0	0	0
	1	21	$175 10^{4}$	4 36	33	2	0	0	0
2	н	22	Total C	Ν	Ο	\mathbf{S}	0	0	0
	11		168 10	1 34	32	1	0	0	0
2	Т	20	Total C	Ν	Ο	\mathbf{S}	0	0	0
	0	20	149 87	32	29	1	0		
2	L	22	Total C	Ν	Ο	\mathbf{S}	0	0	0
			170 103	2 34	33	1	0	0	0
2	Ν	19	Total C	Ν	Ο	\mathbf{S}	0	0	0
	11	10	151 92	31	27	1	0		
2	Р	22	Total C	Ν	Ο	\mathbf{S}	0	0	0
	-		169 103	2 34	32	1	0	· · · · · ·	
2	B	19	Total C	Ν	Ο	\mathbf{S}	0	0	0
	10	10	149 90	31	27	1	0		
2	Т	21	Total C	Ν	Ο	\mathbf{S}	0	0	0
		<u>~1</u>	160 97	32	30	1	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	90	GLY	-	expression tag	UNP Q16611
В	91	GLY	-	expression tag	UNP Q16611
В	92	CYS	-	expression tag	UNP Q16611



Chain	Residue	Modelled	Actual	Comment	Reference
D	90	GLY	-	expression tag	UNP Q16611
D	91	GLY	-	expression tag	UNP Q16611
D	92	CYS	-	expression tag	UNP Q16611
F	90	GLY	-	expression tag	UNP Q16611
F	91	GLY	-	expression tag	UNP Q16611
F	92	CYS	-	expression tag	UNP Q16611
Н	90	GLY	-	expression tag	UNP Q16611
Н	91	GLY	-	expression tag	UNP Q16611
Н	92	CYS	-	expression tag	UNP Q16611
J	90	GLY	-	expression tag	UNP Q16611
J	91	GLY	-	expression tag	UNP Q16611
J	92	CYS	-	expression tag	UNP Q16611
L	90	GLY	-	expression tag	UNP Q16611
L	91	GLY	-	expression tag	UNP Q16611
L	92	CYS	-	expression tag	UNP Q16611
N	90	GLY	-	expression tag	UNP Q16611
N	91	GLY	-	expression tag	UNP Q16611
N	92	CYS	-	expression tag	UNP Q16611
Р	90	GLY	-	expression tag	UNP Q16611
Р	91	GLY	-	expression tag	UNP Q16611
Р	92	CYS	-	expression tag	UNP Q16611
R	90	GLY	-	expression tag	UNP Q16611
R	91	GLY	-	expression tag	UNP Q16611
R	92	CYS	-	expression tag	UNP Q16611
Т	90	GLY	_	expression tag	UNP Q16611
Т	91	GLY	-	expression tag	UNP Q16611
Т	92	CYS	-	expression tag	UNP Q16611

• Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cu 1 1	0	0
3	С	1	Total Cu 1 1	0	0
3	Ε	1	Total Cu 1 1	0	0
3	G	1	Total Cu 1 1	0	0
3	Ι	1	Total Cu 1 1	0	0
3	М	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	О	1	Total Cu 1 1	0	0
3	Q	1	Total Cu 1 1	0	0
3	S	1	Total Cu 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Λ	1	Total O S	0	0
4	A	1	$5 \ 4 \ 1$	0	0
4	С	1	Total O S	0	0
4	G	1	$5 \ 4 \ 1$	0	0
4	Ц	1	Total O S	0	0
4	11	1	$5 \ 4 \ 1$	0	0
4	Ц	1	Total O S	0	0
4	11	1	$5 \ 4 \ 1$	0	0
4	М	1	Total O S	0	0
4	111	T	5 4 1	0	0
4	М	1	Total O S	0	0
4	111	T	$5 \ 4 \ 1$	0	0
	р	1	Total O S	0	0
±	L	1	$5 \ 4 \ 1$	0	0
4	Т	1	Total O S	0	0
<u>+</u>		1	5 4 1	0	



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: Bcl-2 homologous antagonist/killer







• Molecule 1: Bcl-2 homologous antagonist/killer



• Molecule 1: Bcl-2 homologous antagonist/killer





• Molecule 1: Bcl-2 homologous antagonist/killer



• Molecule 1: Bcl-2 homologous antagonist/killer



• Molecule 1: Bcl-2 homologous antagonist/killer



• Molecule 2: Bcl-2 homologous antagonist/killer



Chain B:	68%		20%	12%
868 174 175 177 185 185 185 185 185 188 188 188 188 188	2			
• Molecule 2: Bcl-	2 homologous antagor	nist/killer		
Chain D:	40%	28%	32	%
SER SER T7 0 17 675 675 675 178 178 181 181 183 183 184	ARG ARG TARG TARG CLY CLY CUS			
• Molecule 2: Bcl-	2 homologous antagor	nist/killer		
Chain F:	84%			12% •
SER 869 675 675 75 75 75 75 75 75 75 75 75 75 75 75 7				
• Molecule 2: Bcl-	2 homologous antagor	m nist/killer		
Chain H:	76%		12%	12%
868 672 675 675 675 612 612 612 612 70 612 7				
• Molecule 2: Bcl-	2 homologous antagor	nist/killer		
Chain J:	76%		·	20%
SER 869 775 675 675 617 617 718 617 718 718 617 718 718 718 718 718 718 718 718 718 7				
• Molecule 2: Bcl-	2 homologous antagor	m hist/killer		
Chain L:	64%		24%	12%
S68 M71 G72 G75 G75 G75 G75 G17 G17 G17 G17 G17	25			
• Molecule 2: Bcl-	2 homologous antagor	m hist/killer		
Chain N:	56%	20%		24%
SER SER THR THR 75 075 180 180 180 180 180				
• Molecule 2: Bcl-	2 homologous antagor	m hist/killer		

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Chain P:	60%	24%	• 12%
868 869 77 77 775 775 775 775 775 775 775 775	CYS		
• Molecule 2: Bcl	-2 homologous antagonist/kille	r	
Chain R:	60%	16%	24%
SER SER THR MT1 073 073 073 073 073 073 073 075 017 017 017 017 017			
• Molecule 2: Bcl	-2 homologous antagonist/kille	r	
Chain T:	56%	28%	16%
SER S69 T70 T70 072 073 075 075 077 077 181	Y89 GLY CYS		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	89.39Å 132.22Å 89.38Å	Deneriten
a, b, c, α , β , γ	90.00° 119.20° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	29.34 - 3.06	Depositor
Resolution (A)	29.34 - 3.06	EDS
% Data completeness	90.8 (29.34-3.06)	Depositor
(in resolution range)	90.8(29.34-3.06)	EDS
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.42 (at 3.05 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D	0.213 , 0.249	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.213 , 0.250	DCC
R_{free} test set	2029 reflections $(6.56%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 35.2	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
	0.000 for l,k,-h-l	
	0.000 for -h-l,k,h	
Estimated twinning fraction	0.014 for -h-l,-k,l	Xtriage
	0.019 for h,-k,-h-l	
	0.030 for l,-k,h	
F_o, F_c correlation	0.92	EDS
Total number of atoms	13528	wwPDB-VP
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: CU, $\mathrm{SO4}$

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/1240	0.46	0/1676	
1	С	0.27	0/1245	0.48	0/1683	
1	Е	0.26	0/1290	0.45	0/1746	
1	G	0.36	0/1150	0.46	0/1551	
1	Ι	0.26	0/1183	0.47	0/1595	
1	K	0.26	0/1213	0.44	0/1640	
1	М	0.27	0/1228	0.47	0/1661	
1	0	0.37	0/1235	0.45	0/1669	
1	Q	0.28	0/1231	0.46	0/1664	
1	S	0.36	0/1168	0.50	2/1577~(0.1%)	
2	В	0.30	0/164	0.50	0/219	
2	D	0.27	0/117	0.48	0/155	
2	F	0.27	0/175	0.41	0/231	
2	Н	0.26	0/168	0.44	0/224	
2	J	0.23	0/148	0.40	0/196	
2	L	0.24	0/170	0.42	0/226	
2	N	0.26	0/151	0.41	0/200	
2	Р	0.28	0/169	0.49	0/224	
2	R	0.28	0/149	0.44	0/198	
2	Т	0.27	0/160	0.49	0/213	
All	All	0.30	0/13754	0.46	2/18548~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	S	106	ASN	N-CA-C	-7.15	91.69	111.00
1	S	106	ASN	CB-CA-C	5.37	121.14	110.40

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	А	1213	0	1137	17	0
1	С	1216	0	1149	22	0
1	Ε	1260	0	1195	10	0
1	G	1123	0	1054	9	0
1	Ι	1159	0	1089	9	0
1	Κ	1185	0	1106	15	0
1	М	1201	0	1132	17	0
1	0	1209	0	1121	9	0
1	Q	1199	0	1130	9	0
1	S	1140	0	1060	7	0
2	В	164	0	159	6	0
2	D	119	0	104	5	0
2	F	175	0	166	2	0
2	Н	168	0	162	3	0
2	J	149	0	142	1	0
2	L	170	0	170	6	0
2	Ν	151	0	153	4	0
2	Р	169	0	169	5	0
2	R	149	0	143	5	0
2	Т	160	0	156	5	0
3	А	1	0	0	0	0
3	С	1	0	0	0	0
3	Е	1	0	0	0	0
3	G	1	0	0	0	0
3	Ι	1	0	0	0	0
3	М	1	0	0	0	0
3	0	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
4	А	5	0	0	0	0
4	G	5	0	0	0	0
4	Н	10	0	0	0	0
4	М	10	0	0	0	0
4	Р	5	0	0	0	0
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Т	5	0	0	0	0
All	All	13528	0	12697	125	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 5.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:Q:62:THR:O	1:Q:63:LEU:HD22	1.76	0.83
1:A:80:ILE:HG23	1:K:178:VAL:HG23	1.65	0.78
1:M:32:GLU:OE1	1:M:36:ARG:NH2	2.20	0.75
1:I:117:SER:HB2	2:J:75:GLY:HA3	1.68	0.74
1:K:117:SER:HB2	2:L:75:GLY:HA3	1.71	0.72
1:O:117:SER:HB2	2:P:75:GLY:HA3	1.72	0.72
1:A:117:SER:HB2	2:B:75:GLY:HA3	1.73	0.71
1:E:117:SER:HB2	2:F:75:GLY:HA3	1.73	0.70
1:G:117:SER:HB2	2:H:75:GLY:HA3	1.72	0.70
1:Q:117:SER:HB2	2:R:75:GLY:HA3	1.75	0.69
1:S:38:TYR:OH	1:S:42:ARG:NH1	2.27	0.68
1:M:117:SER:HB2	2:N:75:GLY:HA3	1.77	0.67
1:I:152:GLY:O	1:I:156:ARG:HG2	1.95	0.66
1:K:38:TYR:OH	1:K:42:ARG:NH1	2.30	0.65
1:C:93:PHE:HB3	1:C:137:ARG:NH1	2.12	0.65
1:S:117:SER:HB2	2:T:75:GLY:HA3	1.79	0.64
1:C:117:SER:HB2	2:D:75:GLY:HA3	1.81	0.62
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.66	0.61
1:M:101:GLN:NE2	1:M:105:GLU:HB3	2.17	0.60
1:M:81:ILE:HG22	1:M:185:ASN:HA	1.83	0.60
1:K:32:GLU:OE1	1:K:36:ARG:NH2	2.35	0.59
1:M:38:TYR:OH	1:M:42:ARG:NH1	2.35	0.59
1:E:38:TYR:OH	1:E:42:ARG:NH1	2.35	0.59
1:G:38:TYR:OH	1:G:42:ARG:NH1	2.37	0.58
1:M:101:GLN:HE21	1:M:105:GLU:HB3	1.67	0.58
1:A:149:GLY:O	1:C:36:ARG:NH2	2.36	0.58
1:C:38:TYR:OH	1:C:42:ARG:NH1	2.37	0.57
1:O:32:GLU:OE1	1:O:36:ARG:NH2	2.37	0.56
1:Q:38:TYR:OH	1:Q:42:ARG:NH1	2.37	0.56
1:A:85:ILE:HG13	2:B:85:ILE:HG12	1.87	0.56
1:A:93:PHE:HB3	1:A:137:ARG:HD2	1.88	0.56
1:I:121:SER:OG	1:I:127:ARG:NH1	2.33	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:152:GLY:0	1:O:156:ARG:HD3	2.05	0.56
1:G:92:GLU:O	1:G:96:MET:HG3	2.05	0.55
1:Q:36:ARG:NH1	1:Q:63:LEU:HD11	2.22	0.55
1:E:63:LEU:HD11	1:E:151:LEU:HD21	1.88	0.54
1:O:38:TYR:OH	1:O:42:ARG:NH1	2.40	0.54
1:A:92:GLU:HG2	2:B:77:GLN:HE21	1.72	0.54
1:C:92:GLU:O	1:C:96:MET:HG3	2.08	0.54
1:K:32:GLU:OE2	1:K:156:ARG:NH2	2.41	0.53
1:C:93:PHE:HB3	1:C:137:ARG:HH12	1.72	0.53
1:S:92:GLU:O	1:S:96:MET:HG3	2.09	0.53
1:Q:36:ARG:HH11	1:Q:63:LEU:HD11	1.74	0.53
1:K:92:GLU:O	1:K:96:MET:HG3	2.10	0.52
1:S:117:SER:OG	2:T:72:GLY:HA2	2.09	0.52
1:A:38:TYR:OH	1:A:42:ARG:NH1	2.44	0.51
1:M:41:TYR:O	1:M:45:GLN:HG2	2.11	0.51
1:K:93:PHE:HB3	1:K:137:ARG:HD3	1.93	0.51
1:A:153:GLN:OE1	1:C:62:THR:HB	2.11	0.50
1:M:88:ARG:NH2	2:N:84:ASP:OD2	2.44	0.50
1:0:41:TYR:0	1:O:45:GLN:HG2	2.12	0.50
1:M:121:SER:OG	1:M:127:ARG:NH1	2.41	0.50
1:G:78:LEU:HD22	1:G:129:VAL:HG22	1.94	0.50
1:A:170:TRP:O	1:A:174:ARG:HG2	2.12	0.49
1:E:41:TYR:O	1:E:45:GLN:HG2	2.12	0.49
1:E:117:SER:OG	2:F:72:GLY:HA2	2.12	0.49
1:M:92:GLU:O	1:M:96:MET:HG3	2.13	0.49
1:S:41:TYR:O	1:S:45:GLN:HG2	2.12	0.49
1:C:63:LEU:HG	1:C:65:LEU:HG	1.95	0.49
1:C:89:TYR:OH	2:D:84:ASP:OD2	2.30	0.49
2:R:73:GLN:HG2	2:R:74:VAL:N	2.27	0.48
1:C:88:ARG:HG3	1:C:89:TYR:CD1	2.48	0.48
2:P:68:SER:HG	2:P:69:SER:H	1.61	0.48
1:I:78:LEU:HD22	1:I:129:VAL:HG22	1.96	0.48
2:T:77:GLN:O	2:T:81:ILE:HG22	2.13	0.48
1:Q:117:SER:OG	2:R:72:GLY:HA2	2.14	0.48
1:C:41:TYR:O	1:C:45:GLN:HG2	2.13	0.47
1:S:96:MET:HG2	2:T:74:VAL:HG13	1.96	0.47
1:A:58:PRO:HB3	1:I:146:GLY:HA3	1.96	0.47
1:E:36:ARG:HD3	1:E:63:LEU:HD22	1.95	0.47
1:C:101:GLN:HG3	1:C:102:PRO:HD2	1.97	0.47
1:I:100:LEU:HD23	1:I:141:HIS:HD2	1.79	0.47
1:Q:96:MET:HG3	2:R:74:VAL:HG11	1.96	0.47



	le us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:78:LEU:HD22	1:M:129:VAL:HG22	1.97	0.47
1:M:96:MET:HG2	2:N:74:VAL:HG13	1.97	0.46
1:K:85:ILE:HG13	2:L:85:ILE:HG12	1.98	0.46
1:A:78:LEU:HD22	1:A:129:VAL:HG22	1.96	0.46
1:G:70:THR:O	1:G:70:THR:HG22	2.15	0.46
1:E:78:LEU:HD22	1:E:129:VAL:HG22	1.96	0.45
1:Q:78:LEU:HD22	1:Q:129:VAL:HG22	1.98	0.45
1:A:96:MET:HG3	2:B:74:VAL:HG11	1.97	0.45
1:C:36:ARG:NH1	1:C:64:PRO:HG3	2.31	0.45
1:E:92:GLU:O	1:E:96:MET:HG3	2.16	0.45
2:P:88:ARG:O	2:P:89:TYR:HB2	2.16	0.45
2:D:78:LEU:HA	2:D:81:ILE:HG23	1.98	0.45
1:K:117:SER:OG	2:L:72:GLY:HA2	2.17	0.45
1:0:92:GLU:0	1:O:96:MET:HG3	2.17	0.44
1:C:76:ARG:O	1:C:80:ILE:HD12	2.18	0.44
1:K:110:TYR:HA	2:L:71:MET:SD	2.57	0.44
1:A:147:LEU:HD12	1:C:149:GLY:HA2	1.99	0.44
1:0:117:SER:OG	2:P:72:GLY:HA2	2.17	0.44
1:S:78:LEU:HD22	1:S:129:VAL:HG22	2.00	0.44
1:C:96:MET:HG2	2:D:74:VAL:HG13	1.99	0.43
1:K:96:MET:HG2	2:L:74:VAL:HG13	2.00	0.43
1:A:41:TYR:O	1:A:45:GLN:HG2	2.18	0.43
2:B:77:GLN:HA	2:B:77:GLN:OE1	2.19	0.43
1:O:85:ILE:HG13	2:P:85:ILE:HG12	2.01	0.43
2:D:81:ILE:O	2:D:85:ILE:HG13	2.19	0.42
1:M:42:ARG:HG2	1:M:136:TYR:CE2	2.54	0.42
2:H:88:ARG:HD3	2:H:88:ARG:HA	1.84	0.42
1:I:119:PHE:CD1	1:I:167:ILE:HD11	2.54	0.42
1:C:42:ARG:NH2	1:C:86:ASN:OD1	2.52	0.42
1:I:93:PHE:O	1:I:96:MET:HG2	2.20	0.42
1:A:152:GLY:HA3	1:C:64:PRO:HB2	2.02	0.42
2:T:70:THR:HG22	2:T:73:GLN:CD	2.40	0.42
1:E:104:ALA:HB3	1:E:147:LEU:HD22	2.02	0.42
1:O:125:TRP:CH2	1:O:171:ILE:HG12	2.54	0.42
1:A:102:PRO:HD3	1:M:108:TYR:CZ	2.55	0.42
2:B:88:ARG:HA	2:B:88:ARG:HD2	1.81	0.42
1:K:43:HIS:CE1	1:K:57:ASP:H	2.38	0.42
1:C:80:ILE:HG23	1:G:70:THR:OG1	2.20	0.41
1:K:170:TRP:O	1:K:174:ARG:HG2	2.20	0.41
1:C:73:GLN:HG2	1:C:76:ARG:HH12	1.84	0.41
1:G:117:SER:OG	2:H:72:GLY:HA2	2.20	0.41



Atom-1	Atom-2	Interatomic $distance (Å)$	Clash
		distance (A)	overlap (A)
1:M:81:ILE:HD11	1:M:129:VAL:HG21	2.03	0.41
1:C:77:GLN:HA	1:G:73:GLN:NE2	2.35	0.41
1:K:95:THR:HG21	2:L:68:SER:HB2	2.01	0.41
1:E:63:LEU:C	1:E:65:LEU:H	2.24	0.41
2:N:80:ILE:HD13	2:N:80:ILE:HA	1.87	0.41
1:Q:96:MET:HG3	2:R:74:VAL:CG1	2.51	0.40
1:A:102:PRO:HD3	1:M:108:TYR:CE1	2.57	0.40
1:M:184:CYS:O	1:M:185:ASN:CB	2.68	0.40
1:G:85:ILE:HD13	1:G:85:ILE:HA	1.92	0.40
1:I:77:GLN:O	1:I:81:ILE:HG13	2.22	0.40
1:K:42:ARG:HG2	1:K:136:TYR:CE2	2.56	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	Perce	ntiles
1	А	145/166~(87%)	143 (99%)	2(1%)	0	100	100
1	С	147/166~(89%)	145~(99%)	2(1%)	0	100	100
1	Ε	153/166~(92%)	149 (97%)	3(2%)	1 (1%)	22	52
1	G	135/166~(81%)	132 (98%)	3 (2%)	0	100	100
1	Ι	137/166~(82%)	135~(98%)	1 (1%)	1 (1%)	22	52
1	Κ	141/166~(85%)	139 (99%)	2(1%)	0	100	100
1	М	143/166~(86%)	139~(97%)	4 (3%)	0	100	100
1	Ο	145/166~(87%)	142 (98%)	3~(2%)	0	100	100
1	Q	142/166~(86%)	140 (99%)	2(1%)	0	100	100
1	S	137/166~(82%)	133 (97%)	4 (3%)	0	100	100
2	В	20/25~(80%)	20 (100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	D	15/25~(60%)	14 (93%)	1 (7%)	0	100	100
2	F	22/25~(88%)	22 (100%)	0	0	100	100
2	Н	20/25~(80%)	20 (100%)	0	0	100	100
2	J	18/25~(72%)	18 (100%)	0	0	100	100
2	L	20/25~(80%)	20 (100%)	0	0	100	100
2	Ν	17/25~(68%)	17~(100%)	0	0	100	100
2	Р	20/25~(80%)	19~(95%)	1 (5%)	0	100	100
2	R	17/25~(68%)	17~(100%)	0	0	100	100
2	Т	19/25~(76%)	19 (100%)	0	0	100	100
All	All	1613/1910 (84%)	1583 (98%)	28 (2%)	2(0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ι	101	GLN
1	Е	64	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	123/136~(90%)	123 (100%)	0	100	100	
1	С	125/136~(92%)	124 (99%)	1 (1%)	81	91	
1	Ε	130/136~(96%)	128 (98%)	2(2%)	65	83	
1	G	112/136~(82%)	110 (98%)	2(2%)	59	80	
1	Ι	116/136~(85%)	114 (98%)	2(2%)	60	82	
1	Κ	118/136~(87%)	117~(99%)	1 (1%)	81	91	
1	М	121/136~(89%)	119 (98%)	2(2%)	60	82	
1	Ο	118/136~(87%)	116 (98%)	2(2%)	60	82	
1	Q	122/136~(90%)	118 (97%)	4 (3%)	38	67	



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	S	111/136~(82%)	109~(98%)	2(2%)	59	80
2	В	17/19~(90%)	17 (100%)	0	100	100
2	D	10/19~(53%)	9~(90%)	1 (10%)	7	25
2	F	15/19~(79%)	14 (93%)	1 (7%)	16	43
2	Н	16/19~(84%)	16 (100%)	0	100	100
2	J	14/19~(74%)	14 (100%)	0	100	100
2	L	18/19~(95%)	18 (100%)	0	100	100
2	Ν	15/19~(79%)	14 (93%)	1 (7%)	16	43
2	Р	18/19~(95%)	17 (94%)	1 (6%)	21	49
2	R	13/19~(68%)	13 (100%)	0	100	100
2	Т	15/19~(79%)	15 (100%)	0	100	100
All	All	1347/1550 (87%)	1325 (98%)	22 (2%)	62	83

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All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	156	ARG
2	D	83	ASP
1	Е	84	ASP
1	Е	137	ARG
2	F	87	ARG
1	G	137	ARG
1	G	153	GLN
1	Ι	42	ARG
1	Ι	83	ASP
1	Κ	84	ASP
1	М	84	ASP
1	М	137	ARG
2	Ν	87	ARG
1	0	87	ARG
1	0	137	ARG
2	Р	69	SER
1	Q	87	ARG
1	Q	108[A]	TYR
1	Q	108[B]	TYR
1	Q	156	ARG
1	S	87	ARG
1	S	103	THR



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

Mol	Chain	Res	Type
1	С	77	GLN
1	С	144	GLN
1	G	73	GLN
1	М	101	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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).

Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
INIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	SO4	М	202	-	4,4,4	0.14	0	$6,\!6,\!6$	0.04	0
4	SO4	G	202	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
4	SO4	Н	101	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	Н	102	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	Р	101	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
4	SO4	М	203	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	Т	101	-	4,4,4	0.14	0	6,6,6	0.04	0



There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	151/166~(90%)	-0.47	0 100 100	28, 48, 90, 113	0
1	С	151/166~(90%)	-0.39	1 (0%) 87 72	31,50,81,88	0
1	Е	157/166~(94%)	-0.47	0 100 100	32, 50, 85, 108	0
1	G	139/166~(83%)	-0.32	1 (0%) 87 72	35, 55, 90, 108	0
1	Ι	145/166~(87%)	-0.34	1 (0%) 87 72	36, 55, 99, 129	0
1	Κ	147/166~(88%)	-0.38	0 100 100	36, 54, 78, 118	0
1	М	149/166~(89%)	-0.28	0 100 100	34, 57, 92, 115	0
1	Ο	151/166~(90%)	-0.36	1 (0%) 87 72	31, 54, 94, 115	0
1	Q	147/166~(88%)	-0.28	3 (2%) 65 41	41,66,97,123	0
1	S	143/166~(86%)	-0.10	1 (0%) 87 72	50, 74, 109, 120	0
2	В	22/25~(88%)	-0.59	0 100 100	35, 46, 64, 79	0
2	D	17/25~(68%)	-0.46	0 100 100	50, 59, 78, 79	0
2	F	24/25~(96%)	-0.31	0 100 100	49,60,82,92	0
2	Н	22/25~(88%)	-0.45	0 100 100	34,43,70,98	0
2	J	20/25~(80%)	-0.32	0 100 100	55,68,90,93	0
2	L	22/25~(88%)	-0.31	0 100 100	38,51,69,101	0
2	Ν	19/25~(76%)	-0.24	0 100 100	58, 68, 103, 107	0
2	Р	$2\overline{2}/25~(88\%)$	-0.36	0 100 100	39, 47, 76, 118	0
2	R	19/25~(76%)	-0.11	0 100 100	58, 69, 99, 104	0
2	Т	21/25~(84%)	0.00	0 100 100	59, 73, 96, 106	0
All	All	1688/1910 (88%)	-0.34	8 (0%) 91 79	28, 57, 94, 129	0

All (8) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	G	23	SER	3.6
1	S	49	ALA	3.0
1	Q	62	THR	2.3
1	0	45	GLN	2.2
1	Q	147	LEU	2.1
1	Q	133	GLY	2.1
1	С	181	LEU	2.0
1	Ι	57	ASP	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	SO4	Т	101	5/5	0.86	0.24	114,114,115,116	0
4	SO4	G	202	5/5	0.90	0.31	106,109,115,115	0
4	SO4	М	203	5/5	0.91	0.30	$125,\!126,\!126,\!127$	0
4	SO4	М	202	5/5	0.91	0.20	84,88,90,90	0
3	CU	С	201	1/1	0.93	0.08	60,60,60,60	0
3	CU	0	201	1/1	0.93	0.07	$69,\!69,\!69,\!69$	0
4	SO4	Н	102	5/5	0.94	0.18	68,68,70,71	0
3	CU	М	201	1/1	0.94	0.13	72,72,72,72	0
3	CU	А	201	1/1	0.96	0.12	56, 56, 56, 56	0
3	CU	G	201	1/1	0.97	0.05	49,49,49,49	0
3	CU	Q	201	1/1	0.97	0.04	54,54,54,54	0
4	SO4	А	202	5/5	0.97	0.09	$67,\!68,\!69,\!76$	0
3	CU	Е	201	1/1	0.97	0.06	43,43,43,43	0
3	CU	S	201	1/1	0.99	0.04	62,62,62,62	0
4	SO4	Н	101	5/5	0.99	0.10	39,41,43,46	0
4	SO4	P	101	5/5	0.99	0.12	45,46,48,48	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	CU	Ι	201	1/1	0.99	0.05	$51,\!51,\!51,\!51$	0

6.5 Other polymers (i)

There are no such residues in this entry.

