

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 4, 2024 – 10:04 AM EST

PDB ID	:	8G6D
Title	:	HSV-1 Nuclear Egress Complex (SUP; UL31-R229L)
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Deposited on	:	2023-02-15
Resolution	:	3.92  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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.92 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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		
		100	5%		
1	A	183	75%	15%	10%
	a	100	4%		
1	С	183	70%	20%	• 10%
	-		3%		
1	E	183	73%	17%	10%
	~		7%		
1	G	183	71%	18%	11%
	_		4%		
1	1	183	67%	22%	11%



Mol	Chain	Length	Quality of chain		
1	K	183	4% 73% 16%	•	10%
2	В	260	80%	16%	•••
2	D	260	6%	18%	·
2	F	260	80%	17%	·
2	Н	260	78%	18%	·
2	J	260	6% 75%	20%	·
2	L	260	78%	18%	5%



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## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19341 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	165	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	105	1277	806	231	231	9	0	0	0
1	С	165	Total	С	Ν	0	S	0	0	0
	U	105	1277	806	231	231	9	0	0	0
1	F	165	Total	С	Ν	0	S	0	0	0
		105	1277	806	231	231	9		0	0
1	С	163	Total	С	Ν	0	S	0	0	0
	G		1259	796	226	228	9		0	U
1	т	163	Total	С	Ν	0	S	0	0	0
		105	1259	796	226	228	9		0	0
1	1 IZ	V 164	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	104	1266	800	227	230	9	0	0	U	

• Molecule 1 is a protein called Virion egress protein UL34.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	3	GLY	-	expression tag	UNP P10218
А	4	PRO	-	expression tag	UNP P10218
А	5	LEU	-	expression tag	UNP P10218
А	6	GLY	-	expression tag	UNP P10218
А	7	SER	-	expression tag	UNP P10218
А	8	PRO	-	expression tag	UNP P10218
А	9	GLU	-	expression tag	UNP P10218
А	10	PHE	-	expression tag	UNP P10218
А	11	PRO	-	expression tag	UNP P10218
А	12	GLY	-	expression tag	UNP P10218
А	13	ARG	-	expression tag	UNP P10218
А	14	PRO	-	expression tag	UNP P10218
С	3	GLY	-	expression tag	UNP P10218
С	4	PRO	-	expression tag	UNP P10218
C	5	LEU	-	expression tag	UNP P10218
C	6	GLY	-	expression tag	UNP P10218
C	7	SER	-	expression tag	UNP P10218



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Chain	Residue	Modelled	Actual	Comment	Reference			
С	8	PRO	-	expression tag	UNP P10218			
С	9	GLU	-	expression tag	UNP P10218			
С	10	PHE	-	expression tag	UNP P10218			
С	11	PRO	-	expression tag	UNP P10218			
С	12	GLY	-	expression tag	UNP P10218			
С	13	ARG	-	expression tag	UNP P10218			
С	14	PRO	-	expression tag	UNP P10218			
Е	3	GLY	-	expression tag	UNP P10218			
Е	4	PRO	-	expression tag	UNP P10218			
Е	5	LEU	-	expression tag	UNP P10218			
Е	6	GLY	-	expression tag	UNP P10218			
Е	7	SER	-	expression tag	UNP P10218			
Е	8	PRO	-	expression tag	UNP P10218			
Е	9	GLU	-	expression tag	UNP P10218			
Е	10	PHE	-	expression tag	UNP P10218			
Е	11	PRO	-	expression tag	UNP P10218			
Е	12	GLY	-	expression tag	UNP P10218			
Е	13	ARG	-	expression tag	UNP P10218			
Е	14	PRO	-	expression tag	UNP P10218			
G	3	GLY	-	expression tag	UNP P10218			
G	4	PRO	-	expression tag	UNP P10218			
G	5	LEU	-	expression tag	UNP P10218			
G	6	GLY	-	expression tag	UNP P10218			
G	7	SER	-	expression tag	UNP P10218			
G	8	PRO	-	expression tag	UNP P10218			
G	9	GLU	-	expression tag	UNP P10218			
G	10	PHE	-	expression tag	UNP P10218			
G	11	PRO	-	expression tag	UNP P10218			
G	12	GLY	-	expression tag	UNP P10218			
G	13	ARG	-	expression tag	UNP P10218			
G	14	PRO	-	expression tag	UNP P10218			
Ι	3	GLY	-	expression tag	UNP P10218			
Ι	4	PRO	-	expression tag	UNP P10218			
Ι	5	LEU	-	expression tag	UNP P10218			
Ι	6	GLY	-	expression tag	UNP P10218			
Ι	7	SER	-	expression tag	UNP P10218			
Ι	8	PRO	-	expression tag	UNP P10218			
Ι	9	GLU	-	expression tag	UNP P10218			
Ι	10	PHE	-	expression tag	UNP P10218			
Ι	11	PRO	-	expression tag	UNP P10218			
Ι	12	GLY	-	expression tag	UNP P10218			
Ι	13	ARG	-	expression tag	UNP P10218			

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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	14	PRO	-	expression tag	UNP P10218
K	3	GLY	-	expression tag	UNP P10218
K	4	PRO	-	expression tag	UNP P10218
K	5	LEU	-	expression tag	UNP P10218
K	6	GLY	-	expression tag	UNP P10218
K	7	SER	-	expression tag	UNP P10218
K	8	PRO	-	expression tag	UNP P10218
K	9	GLU	-	expression tag	UNP P10218
K	10	PHE	-	expression tag	UNP P10218
K	11	PRO	-	expression tag	UNP P10218
K	12	GLY	-	expression tag	UNP P10218
K	13	ARG	-	expression tag	UNP P10218
K	14	PRO	-	expression tag	UNP P10218

• Molecule 2 is a protein called Nuclear egress protein 1.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
0	Р	252	Total	С	Ν	0	S	0	0	0
	D	200	1967	1267	335	351	14	0	0	0
0	П	252	Total	С	Ν	0	S	0	0	0
	D	200	1967	1267	335	351	14	0	0	0
0	Б	252	Total	С	Ν	0	S	0	0	0
	Г	200	1967	1267	335	351	14	0	0	U
0	ц	250	Total	С	Ν	0	S	0	0	0
	11	230	1946	1252	332	348	14		0	U
0	т	250	Total	С	Ν	0	S	0	0 0	0
	2 J	200	1943	1252	330	348	13	0		0
9	т	248	Total	С	Ν	0	S	0	0	0
		240	1928	1243	327	344	14	0	0	

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	47	GLY	-	expression tag	UNP P10215
В	48	PRO	-	expression tag	UNP P10215
В	49	GLY	-	expression tag	UNP P10215
В	50	SER	-	expression tag	UNP P10215
В	229	LEU	ARG	conflict	UNP P10215
D	47	GLY	-	expression tag	UNP P10215
D	48	PRO	-	expression tag	UNP P10215
D	49	GLY	-	expression tag	UNP P10215
D	50	SER	-	expression tag	UNP P10215



Chain	Residue	Modelled	Actual	Comment	Reference
D	229	LEU	ARG	conflict	UNP P10215
F	47	GLY	-	expression tag	UNP P10215
F	48	PRO	-	expression tag	UNP P10215
F	49	GLY	-	expression tag	UNP P10215
F	50	SER	-	expression tag	UNP P10215
F	229	LEU	ARG	conflict	UNP P10215
Н	47	GLY	-	expression tag	UNP P10215
Н	48	PRO	-	expression tag	UNP P10215
Н	49	GLY	-	expression tag	UNP P10215
Н	50	SER	-	expression tag	UNP P10215
Н	229	LEU	ARG	conflict	UNP P10215
J	47	GLY	-	expression tag	UNP P10215
J	48	PRO	-	expression tag	UNP P10215
J	49	GLY	-	expression tag	UNP P10215
J	50	SER	-	expression tag	UNP P10215
J	229	LEU	ARG	conflict	UNP P10215
L	47	GLY	-	expression tag	UNP P10215
L	48	PRO	-	expression tag	UNP P10215
L	49	GLY	-	expression tag	UNP P10215
L	50	SER	-	expression tag	UNP P10215
L	229	LEU	ARG	conflict	UNP P10215

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	Н	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O 1 1	0	0
4	J	1	Total O 1 1	0	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: Virion egress protein UL34







 $\bullet$  Molecule 1: Virion egress protein UL34



IN DATA BANK





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	109.56Å 189.10Å 157.10Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $100.52^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	94.55 - 3.92	Depositor
Resolution (A)	94.55 - 3.92	EDS
% Data completeness	97.9 (94.55-3.92)	Depositor
(in resolution range)	84.9 (94.55-3.92)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.88 (at 3.89 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.255 , $0.301$	Depositor
$\Lambda, \Lambda_{free}$	0.256 , $0.303$	DCC
$R_{free}$ test set	1979 reflections $(7.11\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.2	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 27.6	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	19341	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: ZN

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	Bond lengths		angles
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.28	0/1311	0.61	0/1777
1	С	0.27	0/1311	0.58	0/1777
1	Е	0.26	0/1311	0.56	0/1777
1	G	0.28	0/1293	0.55	0/1753
1	Ι	0.28	0/1293	0.57	0/1753
1	Κ	0.26	0/1300	0.55	0/1763
2	В	0.28	0/2019	0.52	0/2750
2	D	0.26	0/2019	0.52	0/2750
2	F	0.27	0/2019	0.55	0/2750
2	Н	0.28	0/1996	0.53	0/2717
2	J	0.27	0/1994	0.55	0/2716
2	L	0.27	0/1978	0.52	0/2694
All	All	0.27	0/19844	0.55	0/26977

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	А	1277	0	1251	20	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1277	0	1251	26	0
1	Е	1277	0	1251	20	0
1	G	1259	0	1231	23	0
1	Ι	1259	0	1231	32	0
1	Κ	1266	0	1238	25	0
2	В	1967	0	1947	30	0
2	D	1967	0	1947	31	0
2	F	1967	0	1947	29	0
2	Н	1946	0	1927	30	0
2	J	1943	0	1924	37	0
2	L	1928	0	1912	34	0
3	В	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	Н	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
All	All	19341	0	19057	299	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 8.

All (299) 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)
2:B:145:VAL:HG12	2:B:269:PRO:HG3	1.55	0.87
2:D:183:PRO:HG3	2:D:268:ILE:HG21	1.59	0.83
1:A:163:GLN:HB3	2:B:102:VAL:HG12	1.65	0.76
1:K:26:ILE:HD12	2:L:79:VAL:HG21	1.70	0.72
1:C:163:GLN:HB3	2:D:102:VAL:HG12	1.72	0.71
1:K:24:ARG:NH2	1:K:28:PRO:O	2.25	0.69
1:G:26:ILE:HG23	2:H:79:VAL:HG11	1.75	0.69
1:C:46:LEU:HD13	1:C:100:PHE:HD2	1.57	0.69
1:G:24:ARG:NH1	1:G:31:LEU:O	2.25	0.69
2:F:122:CYS:SG	2:F:125:CYS:HB2	2.32	0.68
1:G:66:ILE:HG13	1:G:85:LEU:HD12	1.76	0.68
2:B:183:PRO:HG3	2:B:268:ILE:HG21	1.76	0.67
2:B:202:LEU:HD22	2:B:215:LEU:HD21	1.77	0.67
1:C:137:LYS:NZ	1:C:143:ASP:O	2.28	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:70:LEU:HD21	1:G:85:LEU:HG	1.78	0.65
2:J:168:HIS:ND1	2:J:170:ALA:HB2	2.13	0.64
2:B:92:VAL:HG21	2:B:116:LEU:HG	1.79	0.64
1:K:163:GLN:HB3	2:L:102:VAL:HG12	1.79	0.64
1:C:88:GLN:HB2	1:C:125:THR:HG22	1.80	0.63
2:L:167:ARG:NH2	2:L:301:ASP:OD2	2.32	0.63
2:H:209:THR:OG1	2:H:210:TYR:N	2.32	0.63
2:B:261:GLU:O	2:J:302:GLU:HG3	1.98	0.63
2:J:261:GLU:O	2:J:261:GLU:HG3	1.99	0.63
1:C:24:ARG:NH2	1:C:28:PRO:O	2.31	0.62
2:B:145:VAL:CG1	2:B:269:PRO:HG3	2.28	0.62
2:B:141:ILE:O	2:B:145:VAL:HG13	2.00	0.62
1:G:88:GLN:HB2	1:G:125:THR:HG22	1.82	0.61
1:G:86:ARG:NH2	1:G:97:GLN:OE1	2.33	0.61
2:J:203:LEU:HD11	2:J:296:LEU:HB3	1.82	0.60
2:F:279:LYS:O	2:F:283:ILE:HG12	2.02	0.60
2:B:260:ALA:O	2:B:262:LYS:N	2.35	0.59
2:J:104:ASP:O	2:J:105:ASN:ND2	2.35	0.59
2:F:125:CYS:SG	2:F:225:HIS:CE1	2.96	0.58
1:I:103:PRO:O	1:I:105:ASN:N	2.36	0.58
1:G:112:THR:HG22	1:G:115:ARG:HB3	1.85	0.58
1:G:17:GLU:O	1:G:21:GLN:HG3	2.03	0.58
2:J:138:GLU:O	2:J:142:LEU:HG	2.04	0.57
1:E:163:GLN:HB3	2:F:102:VAL:HG22	1.87	0.57
1:A:24:ARG:NH2	1:A:28:PRO:O	2.38	0.57
1:G:87:ILE:HG21	1:G:164:LEU:HD11	1.87	0.57
2:H:158:LEU:O	2:H:162:VAL:HG23	2.05	0.56
2:F:94:LEU:HD22	2:F:114:TYR:CE2	2.40	0.56
2:L:189:HIS:HD2	2:L:202:LEU:HD12	1.70	0.56
1:I:87:ILE:HG21	1:I:164:LEU:HD11	1.87	0.56
2:D:212:GLY:O	2:D:213:HIS:ND1	2.38	0.56
2:B:142:LEU:O	2:B:145:VAL:HG22	2.06	0.55
2:F:114:TYR:OH	1:I:90:THR:O	2.18	0.55
2:D:203:LEU:HD11	2:D:296:LEU:HB3	1.87	0.55
1:A:38:ALA:HB2	1:A:50:CYS:O	2.07	0.55
2:B:243:PHE:HD2	2:B:254:LEU:HD21	1.72	0.55
2:J:268:ILE:O	2:J:268:ILE:HG13	2.06	0.55
2:H:203:LEU:HD11	2:H:296:LEU:HB3	1.89	0.55
1:G:66:ILE:HD12	1:G:153:ILE:HD11	1.88	0.54
1:K:66:ILE:HD13	1:K:85:LEU:HD22	1.88	0.54
2:J:201:ARG:HB2	2:J:218:ILE:HB	1.90	0.54



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:264:THR:HG23	2:J:266:ALA:H	1.71	0.54
2:J:184:GLU:O	2:J:188:VAL:HG23	2.07	0.54
1:I:170:GLY:N	2:J:84:VAL:O	2.38	0.54
2:J:68:LEU:HD21	2:J:78:ILE:HD12	1.89	0.54
1:G:113:PRO:HD3	1:G:136:ILE:HD12	1.90	0.53
2:J:201:ARG:HD2	2:J:296:LEU:HD11	1.89	0.53
1:K:26:ILE:HG23	2:L:79:VAL:HG11	1.90	0.53
1:I:46:LEU:HD11	1:I:76:TRP:HZ3	1.74	0.53
1:I:117:ASN:ND2	2:J:105:ASN:OD1	2.42	0.53
2:L:243:PHE:HB3	2:L:254:LEU:HD11	1.89	0.52
2:F:187:PHE:O	2:F:191:ILE:HG13	2.09	0.52
1:I:103:PRO:C	1:I:105:ASN:H	2.13	0.52
1:G:87:ILE:HD11	1:G:153:ILE:HD13	1.92	0.52
1:E:88:GLN:HG3	1:E:125:THR:HG22	1.92	0.52
1:G:25:LEU:HD21	2:H:76:ILE:HD11	1.92	0.52
1:I:172:GLU:HG2	2:J:84:VAL:CG2	2.40	0.52
1:E:89:ASN:ND2	1:E:121:GLY:O	2.43	0.52
1:K:56:GLY:O	1:K:93:SER:OG	2.16	0.52
1:A:114:GLU:HG3	1:K:49:ARG:HH12	1.75	0.51
2:L:203:LEU:HD11	2:L:296:LEU:HB3	1.92	0.51
1:A:26:ILE:HD13	1:A:68:TYR:CE1	2.45	0.51
2:F:109:LEU:HD22	2:F:114:TYR:HD2	1.76	0.51
1:K:111:ILE:HG21	1:K:166:PHE:CG	2.45	0.51
1:E:145:ARG:HB2	1:E:148:MET:HG3	1.92	0.51
1:A:19:LEU:HD11	1:A:72:LEU:HG	1.92	0.51
2:B:156:ALA:HB1	2:B:293:TYR:OH	2.11	0.51
1:C:119:ILE:HD12	1:C:163:GLN:HG2	1.92	0.51
2:D:158:LEU:O	2:D:162:VAL:HG23	2.11	0.51
1:C:90:THR:O	2:H:114:TYR:OH	2.26	0.51
1:I:56:GLY:O	1:I:93:SER:HB2	2.10	0.51
2:D:203:LEU:HD12	2:D:218:ILE:HD11	1.93	0.51
2:H:136:SER:O	2:H:140:LEU:HG	2.10	0.51
1:I:61:ASP:OD2	1:I:158:ARG:NH2	2.43	0.51
2:H:202:LEU:HG	2:H:215:LEU:HD11	1.92	0.50
2:L:185:LEU:HD22	2:L:215:LEU:HD23	1.93	0.50
2:H:265:ASP:OD1	2:H:266:ALA:N	2.45	0.50
2:L:122:CYS:HB3	2:L:125:CYS:HB2	1.93	0.50
2:D:192:LEU:HD23	2:D:230:LEU:HD23	1.92	0.50
1:G:22:ARG:NH1	2:H:69:ALA:HB2	2.26	0.50
1:C:116:THR:OG1	1:C:166:PHE:O	2.29	0.50
1:C:86:ARG:NH2	1:C:88:GLN:OE1	2.40	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:196:GLY:N	2:F:199:ASP:HB2	2.27	0.50
1:I:26:ILE:HG23	2:J:79:VAL:HG21	1.94	0.50
2:D:203:LEU:O	2:D:215:LEU:HD12	2.12	0.50
1:I:153:ILE:HG12	1:I:166:PHE:HD1	1.77	0.50
2:F:250:SER:HB3	1:I:92:VAL:HG23	1.92	0.50
2:J:94:LEU:HD12	2:J:114:TYR:CZ	2.47	0.50
2:H:138:GLU:O	2:H:142:LEU:HG	2.11	0.49
2:J:182:GLN:OE1	2:J:241:TYR:OH	2.29	0.49
2:L:109:LEU:HB3	2:L:252:PHE:CE1	2.47	0.49
2:D:128:GLY:HA2	2:D:227:HIS:HE2	1.77	0.49
2:F:171:PRO:HG2	2:F:174:ASP:HB3	1.95	0.49
1:E:24:ARG:NH1	1:E:31:LEU:O	2.46	0.48
1:A:145:ARG:HB2	1:A:148:MET:HG3	1.95	0.48
2:B:135:THR:HG21	2:B:191:ILE:HG12	1.95	0.48
2:F:141:ILE:HG23	2:F:269:PRO:HG3	1.95	0.48
2:J:202:LEU:HB3	2:J:215:LEU:HD11	1.95	0.48
2:D:197:ALA:O	2:D:199:ASP:N	2.46	0.48
1:A:132:ASP:O	1:A:136:ILE:HG12	2.14	0.48
1:K:115:ARG:O	1:K:115:ARG:HG3	2.13	0.48
1:C:46:LEU:HD13	1:C:100:PHE:CD2	2.44	0.48
2:B:191:ILE:HG21	2:B:234:MET:HG3	1.95	0.48
2:D:105:ASN:HD21	2:D:116:LEU:HB3	1.79	0.48
1:C:80:PRO:HA	2:D:55:LEU:HD11	1.95	0.48
1:G:30:THR:HB	1:G:62:GLU:HG3	1.96	0.48
2:L:243:PHE:CD2	2:L:256:VAL:HG22	2.49	0.47
2:J:158:LEU:O	2:J:162:VAL:HG23	2.14	0.47
2:B:135:THR:HG22	2:B:140:LEU:HD21	1.95	0.47
2:F:142:LEU:O	2:F:145:VAL:HG12	2.15	0.47
2:J:135:THR:O	2:J:135:THR:OG1	2.33	0.47
1:G:22:ARG:HD3	1:G:72:LEU:HD21	1.97	0.47
1:K:26:ILE:HD11	2:L:75:GLU:HG2	1.97	0.47
2:D:218:ILE:HD13	2:D:253:VAL:HG23	1.96	0.47
1:K:24:ARG:NH1	1:K:31:LEU:O	2.44	0.46
2:L:158:LEU:HB3	2:L:280:MET:SD	2.55	0.46
1:E:56:GLY:O	1:E:93:SER:HB2	2.15	0.46
2:F:201:ARG:NE	2:F:292:GLU:OE2	2.46	0.46
2:L:216:TYR:CD1	2:L:255:VAL:HG22	2.50	0.46
1:A:123:THR:O	1:A:123:THR:HG22	2.15	0.46
2:B:207:ASP:HB3	2:B:210:TYR:O	2.16	0.46
2:D:137:ARG:HA	2:D:140:LEU:HD12	1.97	0.46
2:J:291:LEU:HD21	2:J:295:ARG:HH21	1.81	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:23:ILE:O	1:I:27:VAL:HG23	2.14	0.46
1:A:170:GLY:HA3	2:B:86:LEU:HD21	1.98	0.46
2:B:135:THR:HB	2:B:233:ARG:HG3	1.98	0.46
2:H:151:ILE:HG21	2:H:283:ILE:HD13	1.98	0.46
2:L:255:VAL:HG21	2:L:306:PRO:HD2	1.97	0.46
1:E:90:THR:OG1	1:E:93:SER:O	2.25	0.46
1:I:17:GLU:O	1:I:21:GLN:HG3	2.16	0.46
1:K:22:ARG:NH1	2:L:69:ALA:HB2	2.30	0.46
2:L:217:VAL:HB	2:L:254:LEU:HB3	1.98	0.46
1:K:41:TYR:CE2	1:K:47:PRO:HB3	2.51	0.46
2:L:172:LEU:HD21	2:L:280:MET:HE1	1.98	0.46
2:H:260:ALA:O	2:H:263:PRO:HD3	2.16	0.45
2:J:162:VAL:HA	2:J:172:LEU:HD21	1.97	0.45
2:F:111:GLY:O	1:I:90:THR:HG21	2.17	0.45
1:K:38:ALA:HB1	1:K:47:PRO:HG3	1.98	0.45
1:A:19:LEU:HD13	1:A:76:TRP:HB2	1.99	0.45
1:G:163:GLN:HB3	2:H:102:VAL:HG12	1.98	0.45
1:A:123:THR:HG21	2:J:94:LEU:O	2.17	0.45
1:E:32:ARG:O	1:E:55:HIS:ND1	2.50	0.45
2:L:151:ILE:HD11	2:L:280:MET:HG3	1.99	0.45
2:L:215:LEU:HG	2:L:256:VAL:HB	1.99	0.45
2:B:192:LEU:HD13	2:B:217:VAL:HG11	1.99	0.45
2:J:164:LEU:HD13	2:J:297:TYR:CZ	2.52	0.45
2:D:172:LEU:HD21	2:D:280:MET:HE1	1.99	0.45
2:D:191:ILE:HG21	2:D:234:MET:HG3	1.99	0.45
1:E:88:GLN:HG2	1:E:90:THR:H	1.82	0.45
2:H:201:ARG:HB2	2:H:218:ILE:HB	1.98	0.45
2:F:227:HIS:HB3	2:F:230:LEU:HB2	1.98	0.45
2:H:163:VAL:HG11	2:H:293:TYR:HB3	1.99	0.45
1:K:113:PRO:HD3	1:K:136:ILE:HG12	1.99	0.45
2:L:202:LEU:HD23	2:L:217:VAL:HA	1.99	0.45
1:A:111:ILE:HD13	1:A:128:LEU:HD22	1.99	0.45
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.85	0.44
1:K:85:LEU:HD23	1:K:87:ILE:HD11	1.98	0.44
2:F:109:LEU:HD22	2:F:114:TYR:CD2	2.52	0.44
2:H:141:ILE:HG12	2:H:268:ILE:HG12	1.98	0.44
1:C:26:ILE:HD12	2:D:79:VAL:HG21	1.98	0.44
2:J:141:ILE:O	2:J:145:VAL:HG22	2.17	0.44
1:E:89:ASN:HB2	1:E:120:LEU:HB3	2.00	0.44
2:L:180:LEU:HD13	2:L:271:VAL:HG23	1.98	0.44
2:H:140:LEU:HD13	2:H:187:PHE:HB3	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:46:LEU:HG	1:I:100:PHE:CZ	2.53	0.44
1:I:153:ILE:HG12	1:I:166:PHE:CD1	2.52	0.44
2:H:163:VAL:O	2:H:167:ARG:HG2	2.18	0.44
1:I:89:ASN:C	1:I:91:GLY:H	2.20	0.44
1:G:24:ARG:NH2	1:G:28:PRO:O	2.46	0.44
2:H:203:LEU:O	2:H:215:LEU:HD12	2.18	0.44
1:C:159:MET:HB3	1:C:160:PRO:HD3	1.99	0.43
2:L:209:THR:HG22	2:L:210:TYR:CD1	2.53	0.43
2:L:68:LEU:HD13	2:L:75:GLU:HG3	2.00	0.43
2:L:247:VAL:HG12	2:L:252:PHE:CD1	2.54	0.43
1:C:146:PRO:HG3	2:D:61:TYR:CE1	2.54	0.43
2:D:204:PHE:CE1	2:D:215:LEU:HD13	2.53	0.43
2:J:192:LEU:HD13	2:J:217:VAL:HG11	1.99	0.43
2:J:227:HIS:CD2	2:J:229:LEU:HB2	2.53	0.43
2:H:107:LEU:HA	2:H:116:LEU:HD23	2.00	0.43
2:F:108:THR:HG22	2:F:225:HIS:HD2	1.83	0.43
1:I:112:THR:OG1	1:I:115:ARG:HB2	2.18	0.43
1:K:165:ALA:HB2	2:L:102:VAL:HG21	2.00	0.43
2:L:92:VAL:HG21	2:L:116:LEU:HG	2.00	0.43
1:C:22:ARG:O	1:C:26:ILE:HG12	2.19	0.43
2:F:88:LYS:HA	2:F:118:ILE:HD12	1.99	0.43
2:H:226:LEU:HB3	2:H:231:ILE:HD11	2.00	0.43
2:D:174:ASP:OD1	2:D:174:ASP:N	2.51	0.43
1:E:87:ILE:HG12	1:E:96:PHE:HD1	1.83	0.43
1:K:145:ARG:HB2	1:K:148:MET:HG3	2.00	0.43
2:F:146:GLN:HG2	2:F:149:ASN:HD21	1.83	0.43
2:H:94:LEU:HD21	2:H:109:LEU:HD21	1.99	0.43
2:J:137:ARG:O	2:J:141:ILE:HG13	2.18	0.43
2:L:216:TYR:HD1	2:L:255:VAL:HG22	1.83	0.43
1:A:173:ASP:OD1	1:A:174:ALA:N	2.51	0.43
1:G:27:VAL:HG11	1:G:54:PHE:CE2	2.54	0.43
2:B:111:GLY:O	1:K:90:THR:HG21	2.19	0.43
2:B:114:TYR:CZ	1:K:90:THR:O	2.72	0.43
2:D:182:GLN:NE2	2:D:213:HIS:O	2.45	0.43
1:E:51:ALA:N	1:E:98:GLY:O	2.40	0.43
2:H:216:TYR:CE1	2:H:255:VAL:HG23	2.54	0.43
2:J:218:ILE:HD13	2:J:253:VAL:HG23	2.01	0.43
1:A:16:PHE:HB2	1:A:41:TYR:CZ	2.54	0.42
1:A:111:ILE:HG22	1:A:111:ILE:O	2.18	0.42
2:B:98:LEU:HD11	2:B:254:LEU:HD11	1.99	0.42
1:C:75:ASP:OD1	2:D:62:ARG:HG3	2.19	0.42



	to ac pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:86:ARG:NH1	1:C:97:GLN:OE1	2.53	0.42
1:E:70:LEU:HD22	1:E:83:PRO:HB2	2.01	0.42
1:E:137:LYS:HE3	1:E:149:ALA:HB3	2.01	0.42
2:H:106:CYS:SG	2:H:122:CYS:HB2	2.59	0.42
2:H:141:ILE:O	2:H:145:VAL:HG23	2.20	0.42
1:K:89:ASN:ND2	1:K:162:VAL:HG23	2.34	0.42
2:B:94:LEU:HD11	2:B:109:LEU:CD2	2.49	0.42
2:B:218:ILE:HD13	2:B:253:VAL:HG23	2.01	0.42
1:E:25:LEU:HD22	2:F:76:ILE:HD11	2.01	0.42
2:H:129:ASP:OD1	2:H:129:ASP:N	2.52	0.42
1:I:86:ARG:HH21	1:I:125:THR:HG21	1.84	0.42
1:I:89:ASN:O	1:I:91:GLY:N	2.48	0.42
1:G:132:ASP:O	1:G:136:ILE:HG12	2.20	0.42
1:I:27:VAL:HG21	1:I:54:PHE:CE2	2.54	0.42
2:J:94:LEU:HD12	2:J:114:TYR:CE2	2.54	0.42
1:K:41:TYR:CD2	1:K:47:PRO:HB3	2.55	0.42
2:L:184:GLU:HA	2:L:187:PHE:CD2	2.54	0.42
2:D:122:CYS:HB3	2:D:125:CYS:HB2	2.01	0.42
1:G:22:ARG:HE	2:H:75:GLU:CD	2.22	0.42
2:L:118:ILE:H	2:L:118:ILE:HG13	1.73	0.42
1:A:157:VAL:HG13	1:A:162:VAL:HG22	2.01	0.42
2:D:141:ILE:O	2:D:145:VAL:HG23	2.20	0.42
1:I:90:THR:HB	1:I:93:SER:O	2.20	0.42
1:I:22:ARG:HD3	1:I:72:LEU:HD21	2.01	0.42
1:I:22:ARG:NH2	2:J:65:PHE:O	2.42	0.42
1:A:24:ARG:HD2	1:A:54:PHE:HE1	1.85	0.41
2:B:74:GLU:O	2:B:78:ILE:HG13	2.20	0.41
1:I:128:LEU:HD11	1:I:132:ASP:HB2	2.02	0.41
2:B:217:VAL:HB	2:B:254:LEU:HB3	2.02	0.41
1:C:137:LYS:HZ3	1:C:149:ALA:HB3	1.84	0.41
1:I:84:TYR:OH	1:I:127:GLY:HA3	2.20	0.41
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.86	0.41
2:B:107:LEU:HA	2:B:116:LEU:HD23	2.01	0.41
2:B:248:TRP:O	2:B:251:THR:OG1	2.25	0.41
1:C:17:GLU:O	1:C:20:VAL:HG12	2.20	0.41
1:C:120:LEU:HD11	1:C:126:THR:HG22	2.02	0.41
2:D:216:TYR:HE1	2:D:255:VAL:HG13	1.86	0.41
2:F:156:ALA:HB1	2:F:293:TYR:OH	2.21	0.41
1:G:50:CYS:SG	1:G:53:GLN:HG3	2.61	0.41
2:L:55:LEU:O	2:L:59:GLN:HG3	2.20	0.41
2:D:54:CYS:O	2:D:58:ARG:NE	2.46	0.41



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:F:192:LEU:HB3	2:F:200:PRO:HG3	2.02	0.41	
1:I:84:TYR:HE1	1:I:86:ARG:HB2	1.85	0.41	
2:L:231:ILE:O	2:L:235:LEU:HG	2.21	0.41	
1:C:110:ALA:HB2	1:C:166:PHE:CD2	2.56	0.41	
1:E:86:ARG:NH1	1:E:97:GLN:OE1	2.53	0.41	
2:F:107:LEU:HD23	2:F:226:LEU:HD12	2.01	0.41	
1:A:75:ASP:OD2	2:B:62:ARG:HA	2.21	0.41	
2:D:262:LYS:HB2	2:D:262:LYS:HE3	1.78	0.41	
1:E:63:SER:HB3	1:E:152:TRP:CE3	2.56	0.41	
1:E:84:TYR:OH	1:E:127:GLY:HA3	2.21	0.41	
2:J:153:GLU:O	2:J:193:ARG:NH1	2.54	0.41	
1:A:111:ILE:HD12	1:A:128:LEU:HB2	2.03	0.41	
1:C:33:GLY:HA3	1:C:54:PHE:HA	2.02	0.41	
1:C:66:ILE:HD12	1:C:85:LEU:HD23	2.03	0.41	
2:D:162:VAL:HA	2:D:172:LEU:HD13	2.03	0.41	
1:G:145:ARG:HB2	1:G:148:MET:HG3	2.03	0.41	
2:L:158:LEU:O	2:L:162:VAL:HG23	2.21	0.41	
2:D:164:LEU:HG	2:D:168:HIS:CE1	2.56	0.41	
2:D:176:LEU:HD21	2:D:276:ILE:HB	2.02	0.41	
1:I:25:LEU:HD23	1:I:25:LEU:HA	1.89	0.41	
2:J:96:PHE:CZ	2:J:116:LEU:HD11	2.56	0.41	
1:K:25:LEU:HB3	2:L:76:ILE:HD11	2.01	0.41	
1:I:111:ILE:HG13	1:I:136:ILE:HD13	2.03	0.40	
1:K:112:THR:O	1:K:115:ARG:HB3	2.21	0.40	
2:F:218:ILE:HD13	2:F:253:VAL:HG23	2.04	0.40	
1:I:170:GLY:HA3	2:J:86:LEU:HD21	2.04	0.40	
2:J:196:GLY:O	2:J:199:ASP:N	2.55	0.40	
1:K:19:LEU:HD11	1:K:72:LEU:HG	2.02	0.40	
2:B:136:SER:O	2:B:140:LEU:HG	2.21	0.40	
1:E:163:GLN:HB3	2:F:102:VAL:HG13	2.03	0.40	
2:H:157:PHE:O	2:H:161:LEU:HG	2.21	0.40	
2:J:102:VAL:HG22	2:J:105:ASN:OD1	2.21	0.40	
1:C:30:THR:HB	1:C:62:GLU:HG3	2.04	0.40	
1:C:70:LEU:HD22	1:C:83:PRO:HB2	2.04	0.40	
1:C:88:GLN:HG2	1:C:90:THR:HG23	2.04	0.40	
2:F:94:LEU:HG	2:F:95:PRO:HA	2.04	0.40	
2:F:201:ARG:HB2	2:F:218:ILE:HB	2.04	0.40	
2:F:203:LEU:O	2:F:215:LEU:HD12	2.21	0.40	
2:H:140:LEU:HB3	2:H:187:PHE:CD1	2.55	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	entiles
1	А	163/183~(89%)	152 (93%)	11 (7%)	0	100	100
1	С	163/183~(89%)	150 (92%)	11 (7%)	2(1%)	13	49
1	Е	163/183~(89%)	152 (93%)	9 (6%)	2(1%)	13	49
1	G	161/183~(88%)	149 (92%)	12 (8%)	0	100	100
1	Ι	161/183~(88%)	149 (92%)	11 (7%)	1 (1%)	25	63
1	Κ	162/183~(88%)	152 (94%)	9 (6%)	1 (1%)	25	63
2	В	251/260~(96%)	236 (94%)	12 (5%)	3~(1%)	13	49
2	D	251/260~(96%)	239~(95%)	11 (4%)	1 (0%)	34	71
2	F	251/260~(96%)	237 (94%)	13 (5%)	1 (0%)	34	71
2	Н	246/260~(95%)	232~(94%)	13 (5%)	1 (0%)	34	71
2	J	248/260~(95%)	228 (92%)	18 (7%)	2(1%)	19	57
2	L	244/260~(94%)	232~(95%)	11 (4%)	1 (0%)	34	71
All	All	2464/2658~(93%)	2308 (94%)	141 (6%)	15 (1%)	25	63

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	261	GLU
2	F	197	ALA
1	Ι	104	HIS
2	D	198	CYS
2	L	261	GLU
2	J	267	GLU
1	Κ	90	THR
2	В	260	ALA
1	Е	108	GLY
2	В	208	PRO
1	Е	114	GLU
2	Н	199	ASP



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Mol	Chain	Res	Type
1	С	160	PRO
1	С	175	GLY
2	J	199	ASP

#### 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	Perce	$\mathbf{ntiles}$
1	А	137/150~(91%)	137~(100%)	0	100	100
1	$\mathbf{C}$	137/150~(91%)	137~(100%)	0	100	100
1	Ε	137/150~(91%)	137~(100%)	0	100	100
1	G	135/150~(90%)	135 (100%)	0	100	100
1	Ι	135/150~(90%)	135 (100%)	0	100	100
1	Κ	136/150~(91%)	136 (100%)	0	100	100
2	В	209/214~(98%)	208 (100%)	1 (0%)	88	93
2	D	209/214~(98%)	209 (100%)	0	100	100
2	F	209/214~(98%)	208 (100%)	1 (0%)	88	93
2	Н	208/214~(97%)	208 (100%)	0	100	100
2	J	206/214~(96%)	205 (100%)	1 (0%)	88	93
2	L	206/214~(96%)	205 (100%)	1 (0%)	88	93
All	All	2064/2184~(94%)	2060 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	122	CYS
2	F	106	CYS
2	J	110	SER
2	L	106	CYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:



Mol	Chain	Res	Type
1	Ι	53	GLN
2	J	259	ASN
2	L	189	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	165/183~(90%)	0.69	9 (5%) 25 2	2	41, 62, 89, 107	0
1	С	165/183~(90%)	0.77	8 (4%) 30 2	6	42, 63, 94, 118	0
1	Е	165/183~(90%)	0.65	6 (3%) 42 3	4	43, 63, 93, 115	0
1	G	163/183~(89%)	0.72	12 (7%) 14	12	40,66,95,111	0
1	Ι	163/183~(89%)	0.67	7 (4%) 35 2	9	41, 61, 93, 112	0
1	K	164/183~(89%)	0.68	7 (4%) 35 2	9	40, 63, 92, 110	0
2	В	253/260~(97%)	0.64	7 (2%) 53 4	2	39, 65, 107, 126	0
2	D	253/260~(97%)	0.64	16 (6%) 20 1	l6	44, 70, 104, 124	0
2	F	253/260~(97%)	0.70	18 (7%) 16	13	44, 70, 106, 128	0
2	Н	250/260~(96%)	0.68	5 (2%) 65 5	6	44, 70, 104, 116	0
2	J	250/260~(96%)	0.73	15 (6%) 21	17	40, 73, 110, 125	0
2	L	248/260~(95%)	0.73	14 (5%) 24 2	21	46, 73, 104, 124	0
All	All	2492/2658~(93%)	0.69	124 (4%) 28	25	39, 67, 103, 128	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	68	LEU	4.4
2	D	130	GLY	4.0
1	А	132	ASP	3.9
2	L	264	THR	3.8
1	А	81	CYS	3.7
2	Н	261	GLU	3.6
2	F	130	GLY	3.4
2	J	133	ALA	3.2
1	Ι	147	MET	3.2
1	А	138	GLY	3.2
2	D	251	THR	3.1



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Mol	Chain	Res	Type	RSRZ		
2	D	287	GLY	3.0		
2	F	134	ALA	3.0		
2	В	134	ALA	2.9		
1	G	173	ASP	2.9		
2	J	276	ILE	2.9		
2	F	108	THR	2.9		
2	В	135	THR	2.9		
2	D	135	THR	2.8		
2	F	270	THR	2.8		
2	J	129	ASP	2.8		
2	L	236	THR	2.8		
1	Κ	53	GLN	2.8		
2	F	133	ALA	2.8		
2	F	147	GLN	2.8		
1	Ι	37	GLU	2.7		
2	F	57	GLU	2.7		
2	D	286	ASP	2.7		
1	Е	78	GLU	2.7		
1	Е	177	THR	2.7		
2	J	270	THR	2.7		
2	D	146	GLN	2.7		
1	С	147	MET	2.7		
1	G	138	GLY	2.7		
1	С	119	ILE	2.7		
2	В	280	MET	2.7		
2	J	269	PRO	2.6		
2	D	267	GLU	2.6		
2	F	129	ASP	2.6		
2	L	280	MET	2.6		
2	D	238	CYS	2.6		
2	F	246	HIS	2.6		
2	Н	107	LEU	2.6		
2	Н	154	HIS	2.6		
1	K	77	ALA	2.6		
2	F	275	ASP	2.6		
1	А	173	ASP	2.6		
1	А	123	THR	2.5		
1	Ι	135	THR	2.5		
2	J	246	HIS	2.5		
1	Е	114	GLU	2.5		
2	В	272	SER	2.5		
2	J	275	ASP	2.5		



Mol	Chain	Res	Type	RSRZ
1	G	135	THR	2.5
1	Е	31	LEU	2.5
2	L	269	PRO	2.4
1	G	137	LYS	2.4
2	J	306	PRO	2.4
2	D	129	ASP	2.4
2	D	192	LEU	2.4
2	L	237	ALA	2.4
2	J	111	GLY	2.4
1	Κ	147	MET	2.4
2	F	121	CYS	2.4
2	L	195	GLY	2.4
1	G	35	ASP	2.3
2	J	262	LYS	2.3
1	C	82	ASN	2.3
2	В	261	GLU	2.3
1	Κ	138	GLY	2.3
2	L	286	ASP	2.3
2	D	220	PRO	2.3
2	L	261	GLU	2.3
2	F	75	GLU	2.2
2	J	134	ALA	2.2
2	L	290	MET	2.2
1	G	76	TRP	2.2
1	Κ	19	LEU	2.2
2	F	138	GLU	2.2
2	L	222	THR	2.2
1	G	38	ALA	2.2
1	G	40	PRO	2.2
1	K	173	ASP	2.2
1	G	116	THR	2.2
2	В	158	LEU	2.2
2	D	147	GLN	2.2
2	D	261	GLU	2.2
1	С	48	SER	2.2
1	А	137	LYS	2.2
1	С	128	LEU	2.2
2	F	195	GLY	2.2
2	J	286	ASP	2.2
1	А	41	TYR	2.1
2	В	159	ALA	2.1
2	D	134	ALA	2.1



Mol	Chain	Res	Type	RSRZ	
2	D	131	ARG	2.1	
1	С	57	HIS	2.1	
2	D	269	PRO	2.1	
2	L	285	PHE	2.1	
2	J	253	VAL	2.1	
1	С	37	GLU	2.1	
2	F	306	PRO	2.1	
1	Ι	100	PHE	2.1	
1	Е	81	CYS	2.1	
2	Н	174	ASP	2.1	
1	А	74	ASN	2.1	
1	Ι	114	GLU	2.0	
1	G	81	CYS	2.0	
2	F	82	LEU	2.0	
2	F	192	LEU	2.0	
1	Е	53	GLN	2.0	
1	K	37	GLU	2.0	
2	J	280	MET	2.0	
1	Ι	137	LYS	2.0	
2	L	107	LEU	2.0	
1	G	51	ALA	2.0	
2	Н	306	PRO	2.0	
1	Ι	111	ILE	2.0	
2	F	260	ALA	2.0	
1	G	58	ASP	2.0	
2	J	217	VAL	2.0	
2	L	263	PRO	2.0	
1	А	147	MET	2.0	
1	С	137	LYS	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
3	ZN	В	401	1/1	0.85	0.08	74,74,74,74	0
3	ZN	Н	401	1/1	0.89	0.24	198,198,198,198	0
3	ZN	F	401	1/1	0.91	0.19	100,100,100,100	0
3	ZN	D	401	1/1	0.96	0.12	121,121,121,121	0
3	ZN	L	401	1/1	0.96	0.17	159,159,159,159	0
3	ZN	J	401	1/1	0.97	0.15	62,62,62,62	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

