



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 12:13 PM EDT

PDB ID : 5JIA  
Title : The Crystal Structure Of IUS-SPRY Domain From RanBP10  
Authors : Hong, S.K.; Kim, K.-H.; Kim, E.E.  
Deposited on : 2016-04-22  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

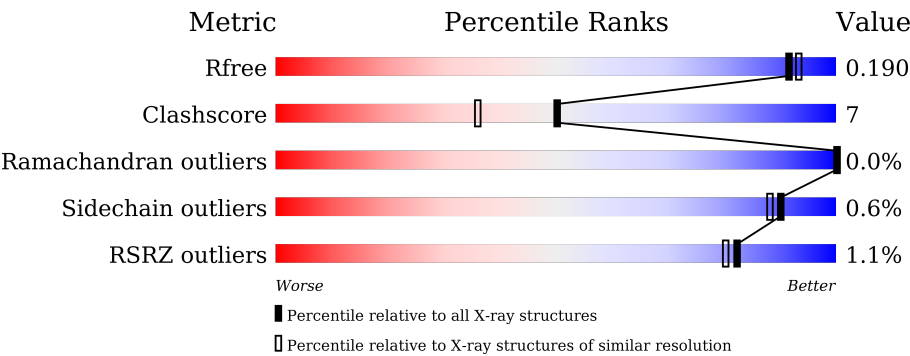
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

# 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 1.80 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.










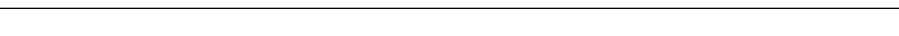
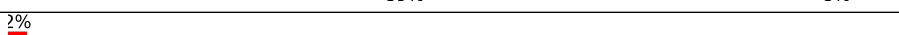
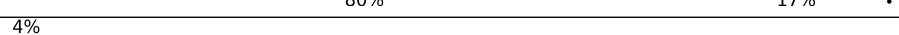
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	210	<div><div></div><div>81%16%..</div></div>
1	B	210	<div><div>%</div><div>88%10%.</div></div>
1	C	210	<div><div>%</div><div>87%10%.</div></div>
1	D	210	<div><div>2%</div><div>86%14%</div></div>
1	E	210	<div><div>%</div><div>87%11%.</div></div>
1	F	210	<div><div></div><div>87%12%.</div></div>

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Mol	Chain	Length	Quality of chain
1	G	210	 88% 9% .
1	H	210	 89% 7% .
1	I	210	 86% 12% .
1	J	210	 85% 10% 5%
1	K	210	 88% 9% .
1	L	210	 93% 5% .
1	M	210	 86% 12% .
1	N	210	 89% 8% .
1	O	210	 80% 17% .
1	P	210	 81% 15% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IMD	A	901	-	-	-	X
2	IMD	D	301	-	-	-	X
2	IMD	E	301	-	-	-	X
2	IMD	H	301	-	-	-	X
2	IMD	J	301	-	-	-	X
2	IMD	N	301	-	-	-	X

## 2 Entry composition

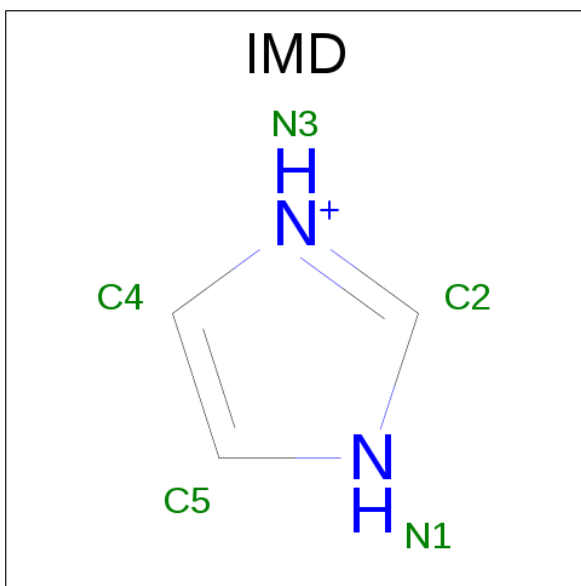
There are 3 unique types of molecules in this entry. The entry contains 27983 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ran-binding protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1614	1021	288	297	8			
1	B	207	Total	C	N	O	S	0	0	0
			1623	1026	289	300	8			
1	C	205	Total	C	N	O	S	0	0	0
			1602	1012	285	297	8			
1	D	210	Total	C	N	O	S	0	0	0
			1640	1036	292	304	8			
1	E	207	Total	C	N	O	S	0	0	0
			1618	1023	288	299	8			
1	F	207	Total	C	N	O	S	0	0	0
			1615	1020	287	300	8			
1	G	203	Total	C	N	O	S	0	0	0
			1586	1003	280	295	8			
1	H	203	Total	C	N	O	S	0	0	0
			1589	1005	283	293	8			
1	I	206	Total	C	N	O	S	0	0	0
			1614	1021	287	298	8			
1	J	199	Total	C	N	O	S	0	0	0
			1550	980	275	287	8			
1	K	203	Total	C	N	O	S	0	0	0
			1586	1003	280	295	8			
1	L	205	Total	C	N	O	S	0	0	0
			1607	1016	286	297	8			
1	M	208	Total	C	N	O	S	0	0	0
			1624	1026	289	301	8			
1	N	203	Total	C	N	O	S	0	0	0
			1586	1003	280	295	8			
1	O	202	Total	C	N	O	S	0	0	0
			1572	992	278	294	8			
1	P	204	Total	C	N	O	S	0	0	0
			1596	1011	284	293	8			

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	E	1	Total	C	N	0	0
			5	3	2		
2	G	1	Total	C	N	0	0
			5	3	2		
2	H	1	Total	C	N	0	0
			5	3	2		
2	J	1	Total	C	N	0	0
			5	3	2		
2	N	1	Total	C	N	0	0
			5	3	2		
2	P	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	130	Total	O	0	0
			130	130		
3	C	141	Total	O	0	0
			141	141		

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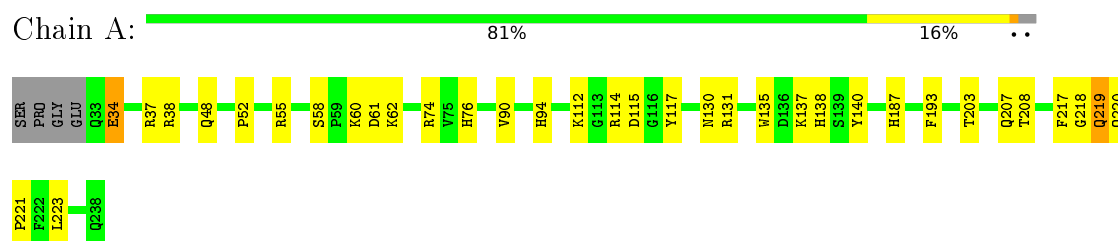
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	137	Total 137	O 137	0	0
3	E	173	Total 173	O 173	0	0
3	F	148	Total 148	O 148	0	0
3	G	153	Total 153	O 153	0	0
3	H	161	Total 161	O 161	0	0
3	I	199	Total 199	O 199	0	0
3	J	155	Total 155	O 155	0	0
3	K	168	Total 168	O 168	0	0
3	L	94	Total 94	O 94	0	0
3	M	165	Total 165	O 165	0	0
3	N	148	Total 148	O 148	0	0
3	O	101	Total 101	O 101	0	0
3	P	79	Total 79	O 79	0	0

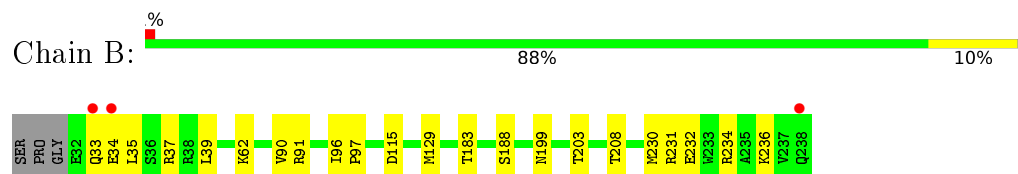
### 3 Residue-property plots

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.

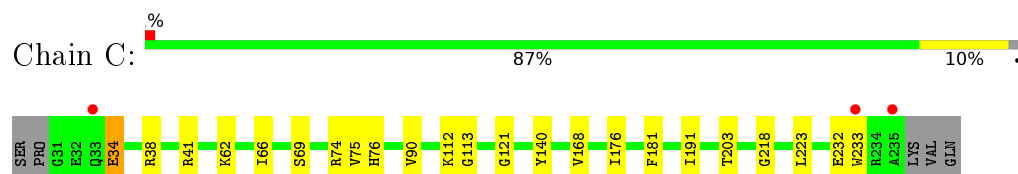
- Molecule 1: Ran-binding protein 10



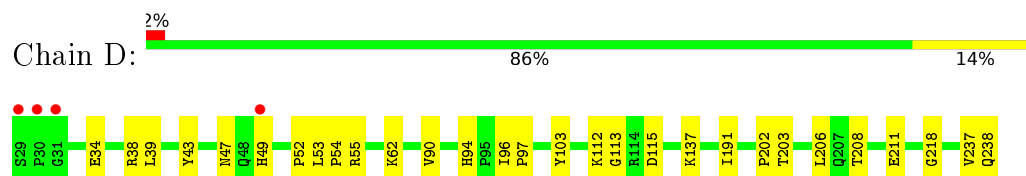
- Molecule 1: Ran-binding protein 10



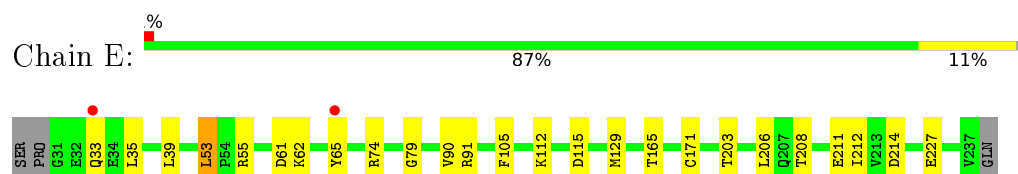
- Molecule 1: Ran-binding protein 10




- Molecule 1: Ran-binding protein 10

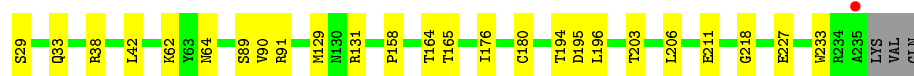


- Molecule 1: Ran-binding protein 10



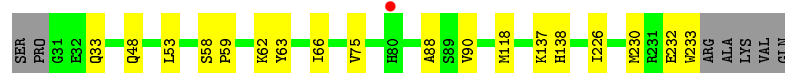
- Molecule 1: Ran-binding protein 10

Chain F:  87% 12%




- Molecule 1: Ran-binding protein 10

Chain G:  88% 9%




- Molecule 1: Ran-binding protein 10

Chain H:  89% 7%




- Molecule 1: Ran-binding protein 10

Chain I:  86% 12%



- Molecule 1: Ran-binding protein 10

Chain J:  85% 10% 5%



- Molecule 1: Ran-binding protein 10

Chain K:  88% 9%



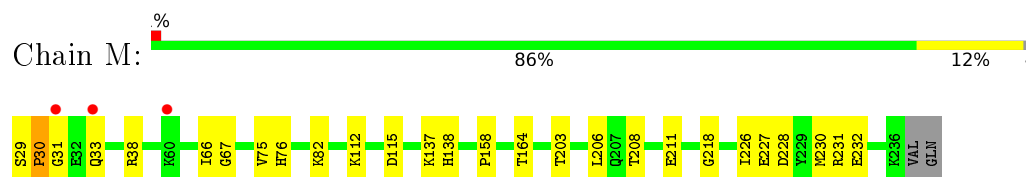
- Molecule 1: Ran-binding protein 10

Chain L:  93% 5%

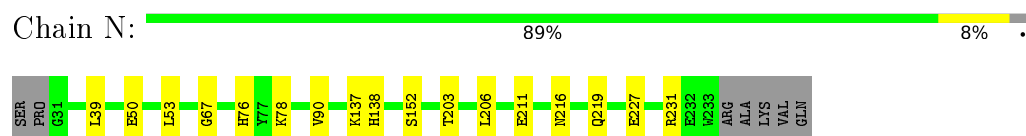




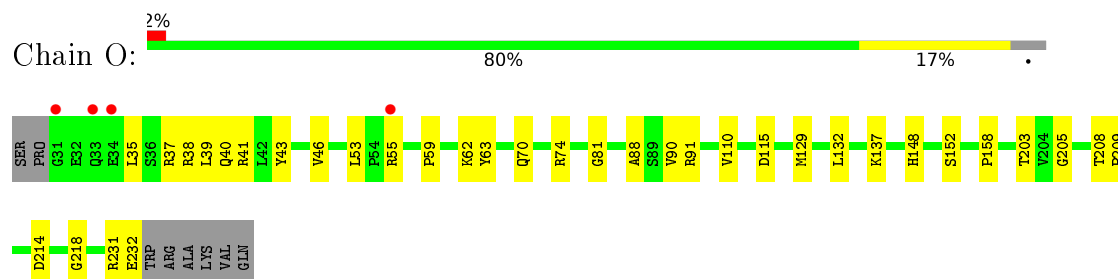
- Molecule 1: Ran-binding protein 10



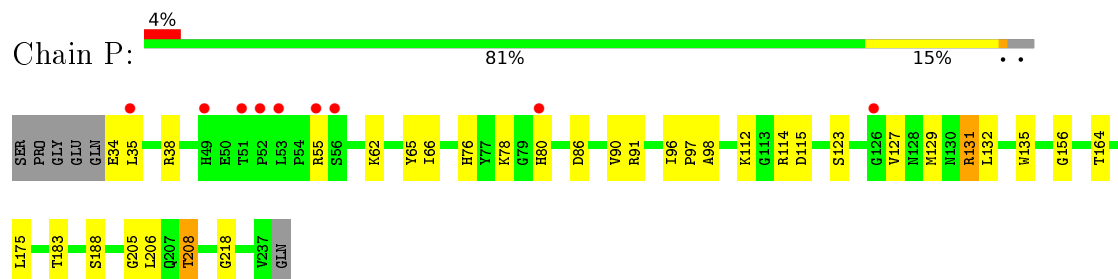
- Molecule 1: Ran-binding protein 10



- Molecule 1: Ran-binding protein 10



- Molecule 1: Ran-binding protein 10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.34Å 79.24Å 157.63Å 90.00° 97.91° 90.00°	Depositor
Resolution (Å)	41.25 – 1.80 41.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (41.25-1.80) 92.6 (41.25-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, $R_{free}$	0.184 , 0.227 0.188 , 0.190	Depositor DCC
$R_{free}$ test set	15427 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5519e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.43	0/1662	0.58	0/2255
1	B	0.39	0/1671	0.58	0/2267
1	C	0.48	1/1650 (0.1%)	0.58	1/2239 (0.0%)
1	D	0.41	0/1689	0.65	0/2292
1	E	0.40	0/1666	0.61	1/2260 (0.0%)
1	F	0.44	0/1664	0.59	0/2259
1	G	0.37	0/1634	0.56	0/2218
1	H	0.40	0/1637	0.57	1/2222 (0.0%)
1	I	0.44	0/1662	0.61	0/2255
1	J	0.42	0/1596	0.61	0/2166
1	K	0.41	0/1634	0.56	0/2218
1	L	0.34	0/1655	0.54	0/2245
1	M	0.44	0/1673	0.60	0/2270
1	N	0.38	0/1634	0.58	0/2218
1	O	0.36	0/1618	0.59	0/2195
1	P	0.38	0/1644	0.62	1/2231 (0.0%)
All	All	0.41	1/26389 (0.0%)	0.59	4/35810 (0.0%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	ARG	CZ-NH2	-5.80	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	131	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	41	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	P	206	LEU	CA-CB-CG	5.11	127.06	115.30
1	E	53	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	64	ASN	Mainchain

## 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	1614	0	1540	30	0
1	B	1623	0	1546	18	0
1	C	1602	0	1519	19	0
1	D	1640	0	1561	29	0
1	E	1618	0	1541	21	0
1	F	1615	0	1531	17	0
1	G	1586	0	1501	12	0
1	H	1589	0	1510	13	0
1	I	1614	0	1538	33	0
1	J	1550	0	1476	21	0
1	K	1586	0	1501	16	0
1	L	1607	0	1529	7	0
1	M	1624	0	1544	23	0
1	N	1586	0	1501	16	0
1	O	1572	0	1491	50	0
1	P	1596	0	1524	33	0
2	A	5	0	5	2	0
2	D	5	0	5	0	0
2	E	5	0	5	0	0
2	G	5	0	5	0	0
2	H	5	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	5	0	5	1	0
2	N	5	0	5	0	0
2	P	5	0	5	1	0
3	A	169	0	0	1	0
3	B	130	0	0	2	0
3	C	141	0	0	1	0
3	D	137	0	0	2	0
3	E	173	0	0	1	0
3	F	148	0	0	0	0
3	G	153	0	0	1	0
3	H	161	0	0	1	0
3	I	199	0	0	4	0
3	J	155	0	0	2	0
3	K	168	0	0	2	0
3	L	94	0	0	1	0
3	M	165	0	0	1	0
3	N	148	0	0	1	0
3	O	101	0	0	2	0
3	P	79	0	0	2	0
All	All	27983	0	24393	349	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 7.

All (349) 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:O:231:ARG:O	1:O:232:GLU:HG2	1.41	1.17
1:I:90:VAL:HA	1:I:129:MET:HE1	1.18	1.17
1:O:231:ARG:O	1:O:232:GLU:CG	1.95	1.14
1:I:90:VAL:HA	1:I:129:MET:CE	1.78	1.12
1:O:40:GLN:HG2	1:O:41:ARG:NH1	1.65	1.12
1:N:137:LYS:HZ3	1:N:138:HIS:CE1	1.67	1.11
1:O:40:GLN:CG	1:O:41:ARG:HH11	1.63	1.09
1:K:60:LYS:HD3	1:M:158:PRO:HG2	1.32	1.07
1:N:137:LYS:NZ	1:N:138:HIS:CE1	2.27	1.02
1:G:232:GLU:OE1	1:G:233:TRP:CD1	2.16	0.98
1:N:216:ASN:HA	1:N:219:GLN:HE22	1.27	0.97
1:O:40:GLN:CG	1:O:41:ARG:NH1	2.25	0.97
1:I:137:LYS:HG2	3:I:422:HOH:O	1.62	0.97
1:O:231:ARG:O	1:O:232:GLU:CD	2.04	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:MET:SD	3:I:464:HOH:O	2.25	0.94
1:M:29:SER:N	1:M:30:PRO:CD	2.35	0.89
1:J:230:MET:O	1:J:231:ARG:HG2	1.71	0.89
1:I:90:VAL:CA	1:I:129:MET:CE	2.50	0.89
1:E:74:ARG:HD3	1:E:214:ASP:OD1	1.71	0.88
1:O:41:ARG:HD3	1:O:41:ARG:N	1.87	0.88
1:O:40:GLN:HG3	1:O:41:ARG:HH11	1.37	0.88
1:O:74:ARG:HG3	1:O:214:ASP:OD1	1.72	0.87
1:K:60:LYS:CD	1:M:158:PRO:HG2	2.07	0.85
1:J:34:GLU:O	1:J:38:ARG:HG3	1.75	0.85
1:P:62:LYS:HB2	1:P:90:VAL:HG12	1.58	0.84
1:G:232:GLU:OE1	1:G:233:TRP:NE1	2.11	0.82
1:K:60:LYS:HD3	1:M:158:PRO:CG	2.09	0.81
1:N:137:LYS:HG3	1:N:138:HIS:CD2	2.16	0.80
1:G:118:MET:SD	3:G:528:HOH:O	2.38	0.80
1:O:232:GLU:OE1	1:O:232:GLU:HA	1.82	0.80
1:E:74:ARG:HH21	1:E:212:ILE:HG21	1.47	0.79
1:D:112:LYS:HE3	1:D:113:GLY:O	1.83	0.78
1:P:123:SER:HB2	1:P:127:VAL:HG11	1.66	0.78
1:O:37:ARG:HG3	1:O:41:ARG:HH21	1.48	0.77
1:P:115:ASP:H	1:P:208:THR:HG21	1.49	0.77
1:D:43:TYR:CD2	1:D:53:LEU:HD11	2.19	0.77
1:O:37:ARG:HG3	1:O:41:ARG:NH2	2.00	0.76
1:P:66:ILE:HG21	1:P:90:VAL:HG11	1.68	0.76
1:C:38:ARG:NH2	1:C:38:ARG:HB3	2.02	0.75
1:N:137:LYS:NZ	1:N:138:HIS:NE2	2.30	0.74
1:O:39:LEU:HD13	1:O:53:LEU:HD12	1.66	0.74
1:A:217:PHE:H	1:A:219:GLN:HE22	1.35	0.74
1:O:70:GLN:CD	1:O:74:ARG:HH21	1.91	0.73
1:M:29:SER:N	1:M:30:PRO:HD2	2.03	0.73
1:N:216:ASN:HA	1:N:219:GLN:NE2	2.02	0.72
1:I:48:GLN:HE22	1:I:55:ARG:HH21	1.38	0.72
1:P:35:LEU:HD21	1:P:55:ARG:CG	2.20	0.71
1:I:91:ARG:N	1:I:129:MET:HE3	2.05	0.71
1:I:62:LYS:HA	1:I:129:MET:HE1	1.72	0.70
1:I:43:TYR:CD2	1:I:53:LEU:HD11	2.26	0.70
1:E:112:LYS:H	1:E:165:THR:HG22	1.56	0.70
1:O:40:GLN:HG2	1:O:41:ARG:HH12	1.53	0.70
1:P:114:ARG:HB3	1:P:208:THR:CG2	2.21	0.70
1:D:96:ILE:HD11	1:D:202:PRO:HG3	1.74	0.70
1:P:35:LEU:HD21	1:P:55:ARG:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.57	0.69
1:P:131:ARG:NH2	3:P:401:HOH:O	2.25	0.69
1:I:48:GLN:NE2	1:I:55:ARG:HH21	1.90	0.69
1:C:69:SER:OG	1:C:76:HIS:HE1	1.74	0.69
1:C:69:SER:OG	1:C:76:HIS:CE1	2.46	0.69
1:E:39:LEU:HD13	1:E:53:LEU:HD12	1.76	0.68
1:J:146:ASP:O	1:J:148:HIS:HD2	1.77	0.67
1:D:206:LEU:HD22	1:D:211:GLU:HB3	1.77	0.67
1:O:70:GLN:NE2	1:O:74:ARG:HH21	1.93	0.67
1:O:70:GLN:NE2	1:O:74:ARG:NH2	2.42	0.67
1:O:55:ARG:HB2	1:O:55:ARG:CZ	2.25	0.67
1:E:65:TYR:CD2	1:E:79:GLY:HA3	2.29	0.66
1:J:114:ARG:NH2	3:J:401:HOH:O	2.28	0.66
1:N:206:LEU:HD22	1:N:211:GLU:HB3	1.78	0.66
1:M:137:LYS:HG2	1:M:138:HIS:CD2	2.31	0.65
1:P:114:ARG:HB3	1:P:208:THR:HG23	1.78	0.65
1:A:203:THR:HG21	3:A:1019:HOH:O	1.95	0.65
1:C:203:THR:HG21	3:C:308:HOH:O	1.95	0.65
1:B:230:MET:O	1:B:234:ARG:HG3	1.96	0.64
1:F:131:ARG:HH12	2:H:301:IMD:HN1	1.44	0.64
1:C:62:LYS:HB3	1:C:90:VAL:HG23	1.79	0.64
1:D:55:ARG:NH1	3:D:402:HOH:O	2.31	0.64
1:J:34:GLU:HG3	1:J:38:ARG:HD2	1.80	0.63
1:C:112:LYS:NZ	1:C:113:GLY:O	2.31	0.63
1:M:206:LEU:HD22	1:M:211:GLU:HB3	1.81	0.62
1:N:137:LYS:HZ1	1:N:138:HIS:CE1	2.18	0.62
1:O:74:ARG:NH2	3:O:302:HOH:O	2.31	0.62
1:E:206:LEU:HD22	1:E:211:GLU:HB3	1.82	0.61
1:H:48:GLN:OE1	1:H:55:ARG:NH1	2.33	0.61
1:J:38:ARG:HD3	1:J:218:GLY:O	2.01	0.61
1:O:70:GLN:HE22	1:O:74:ARG:NH2	1.97	0.61
1:M:227:GLU:O	1:M:231:ARG:HG3	2.01	0.60
1:N:227:GLU:O	1:N:231:ARG:HG3	2.01	0.60
1:O:41:ARG:CD	1:O:41:ARG:N	2.59	0.60
1:E:39:LEU:HB3	1:E:53:LEU:CD1	2.31	0.60
1:O:232:GLU:CA	1:O:232:GLU:OE1	2.48	0.60
1:N:39:LEU:HB3	1:N:53:LEU:HD13	1.84	0.59
1:E:203:THR:HG21	3:E:402:HOH:O	2.02	0.59
1:C:38:ARG:CZ	1:C:38:ARG:HB3	2.33	0.59
1:A:217:PHE:H	1:A:219:GLN:NE2	1.99	0.59
1:D:47:ASN:OD1	1:D:49:HIS:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:TYR:O	1:O:46:VAL:HG12	2.03	0.59
1:P:66:ILE:HG21	1:P:90:VAL:CG1	2.33	0.59
1:J:226:ILE:O	1:J:230:MET:HG3	2.02	0.59
1:I:39:LEU:HD22	1:I:53:LEU:HD12	1.85	0.58
1:D:96:ILE:HD11	1:D:103:TYR:CE2	2.39	0.58
1:A:62:LYS:HB3	1:A:90:VAL:HG23	1.85	0.58
1:M:203:THR:HG21	3:M:303:HOH:O	2.04	0.58
1:P:91:ARG:HG3	1:P:129:MET:CE	2.34	0.58
1:I:90:VAL:CA	1:I:129:MET:HE1	2.10	0.58
1:F:89:SER:C	1:F:129:MET:HE3	2.24	0.58
1:L:62:LYS:HB3	1:L:90:VAL:HG23	1.84	0.58
1:A:60:LYS:HG3	1:A:61:ASP:N	2.19	0.58
1:E:33:GLN:OE1	1:E:33:GLN:N	2.36	0.58
1:A:38:ARG:HD2	1:A:218:GLY:O	2.03	0.58
1:P:131:ARG:HH12	2:P:301:IMD:HN1	1.51	0.58
1:B:62:LYS:HB3	1:B:90:VAL:HG23	1.86	0.57
1:H:33:GLN:HG2	1:H:34:GLU:N	2.19	0.57
1:N:203:THR:HG21	3:N:412:HOH:O	2.03	0.57
1:A:112:LYS:NZ	1:A:114:ARG:O	2.37	0.57
1:G:48:GLN:HE21	1:G:53:LEU:H	1.52	0.57
1:E:35:LEU:HD21	1:E:55:ARG:HB3	1.85	0.57
1:B:199:ASN:ND2	3:B:302:HOH:O	2.31	0.57
1:I:90:VAL:CA	1:I:129:MET:HE2	2.34	0.57
1:J:230:MET:O	1:J:231:ARG:CG	2.48	0.57
1:A:187:HIS:NE2	1:G:33:GLN:NE2	2.53	0.57
1:O:148:HIS:CD2	1:O:158:PRO:HA	2.40	0.56
1:A:130:ASN:C	1:A:131:ARG:HG2	2.25	0.56
1:D:43:TYR:HD2	1:D:53:LEU:HD11	1.70	0.56
1:O:39:LEU:HB3	1:O:53:LEU:CD1	2.36	0.56
1:A:34:GLU:HG3	1:A:37:ARG:NH2	2.21	0.56
1:J:146:ASP:O	1:J:148:HIS:CD2	2.60	0.55
1:I:39:LEU:HD22	1:I:53:LEU:CD1	2.36	0.55
1:C:176:ILE:HD12	1:C:233:TRP:CZ3	2.42	0.55
1:P:91:ARG:HG3	1:P:129:MET:HE1	1.88	0.55
1:C:34:GLU:O	1:C:38:ARG:HG3	2.06	0.54
1:P:115:ASP:N	1:P:208:THR:HG21	2.19	0.54
1:I:203:THR:HG21	3:I:302:HOH:O	2.07	0.54
1:O:37:ARG:HG3	1:O:41:ARG:CZ	2.38	0.54
1:O:41:ARG:HD3	1:O:41:ARG:H	1.66	0.54
1:D:203:THR:HG21	3:D:521:HOH:O	2.07	0.54
1:E:74:ARG:HD2	1:E:212:ILE:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:VAL:O	1:K:203:THR:HG23	2.07	0.54
1:I:114:ARG:HD2	1:I:115:ASP:OD2	2.08	0.54
1:J:34:GLU:CG	1:J:38:ARG:HD2	2.37	0.54
1:C:74:ARG:HG2	1:C:76:HIS:CE1	2.43	0.53
1:M:30:PRO:HG2	1:M:31:GLY:H	1.73	0.53
1:H:62:LYS:HB3	1:H:90:VAL:HG23	1.91	0.53
1:P:35:LEU:O	1:P:38:ARG:HB3	2.07	0.53
1:H:203:THR:HG21	3:H:402:HOH:O	2.08	0.53
1:D:96:ILE:CD1	1:D:103:TYR:CD2	2.91	0.53
1:J:114:ARG:HD2	1:J:115:ASP:OD2	2.08	0.53
1:F:131:ARG:NH1	2:H:301:IMD:HN1	2.06	0.53
1:J:203:THR:HG21	3:J:402:HOH:O	2.08	0.53
1:C:38:ARG:NH2	1:C:38:ARG:CB	2.71	0.53
1:H:33:GLN:HG2	1:H:34:GLU:H	1.73	0.52
1:E:39:LEU:HD13	1:E:53:LEU:CD1	2.38	0.52
1:O:132:LEU:HD23	1:O:205:GLY:HA3	1.90	0.52
1:A:135:TRP:CD2	2:A:901:IMD:H4	2.45	0.52
1:F:176:ILE:HD12	1:F:233:TRP:HE1	1.75	0.52
1:H:115:ASP:HB2	1:H:208:THR:HG21	1.92	0.52
1:J:34:GLU:CD	1:J:38:ARG:HD2	2.30	0.51
1:L:227:GLU:O	1:L:231:ARG:HG3	2.09	0.51
1:O:62:LYS:HB3	1:O:90:VAL:HG23	1.92	0.51
1:D:52:PRO:HG2	1:D:94:HIS:CD2	2.45	0.51
1:E:91:ARG:NH1	1:E:129:MET:SD	2.83	0.51
1:M:228:ASP:O	1:M:232:GLU:HB2	2.10	0.51
1:O:74:ARG:HH11	1:O:110:VAL:HG11	1.75	0.51
1:A:60:LYS:HG3	1:A:61:ASP:H	1.75	0.51
1:J:62:LYS:HB3	1:J:90:VAL:HG23	1.91	0.51
1:O:39:LEU:HD13	1:O:53:LEU:CD1	2.40	0.51
1:P:65:TYR:O	1:P:78:LYS:N	2.44	0.50
1:O:38:ARG:HD2	1:O:218:GLY:O	2.11	0.50
1:F:164:THR:OG1	1:F:165:THR:N	2.43	0.50
1:A:52:PRO:HG2	1:A:94:HIS:CD2	2.46	0.50
1:I:43:TYR:HD2	1:I:53:LEU:HD11	1.71	0.50
1:I:48:GLN:HE22	1:I:55:ARG:NH2	2.07	0.50
1:D:96:ILE:HD13	1:D:103:TYR:CD2	2.46	0.50
1:I:91:ARG:N	1:I:129:MET:CE	2.73	0.50
1:D:191:ILE:HD11	1:N:50:GLU:HG2	1.92	0.50
1:J:115:ASP:HB2	1:J:208:THR:HG21	1.94	0.50
1:K:129:MET:SD	3:K:431:HOH:O	2.59	0.50
1:O:39:LEU:HD22	1:O:53:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:80:HIS:HB2	1:P:86:ASP:OD2	2.12	0.50
1:G:63:TYR:HB3	1:G:88:ALA:HB1	1.93	0.49
1:O:37:ARG:HG3	1:O:41:ARG:NE	2.27	0.49
1:N:67:GLY:HA3	1:N:78:LYS:HE3	1.93	0.49
1:O:35:LEU:HD21	1:O:55:ARG:HH21	1.76	0.49
1:E:61:ASP:OD1	1:E:91:ARG:NH2	2.45	0.49
1:P:98:ALA:HA	1:P:175:LEU:HG	1.94	0.49
1:P:183:THR:HG22	1:P:188:SER:HA	1.95	0.49
1:B:232:GLU:HG3	1:B:236:LYS:HD2	1.94	0.49
1:P:131:ARG:NH2	1:P:135:TRP:CE3	2.81	0.49
1:A:117:TYR:OH	1:M:82:LYS:NZ	2.46	0.48
1:L:115:ASP:HB2	1:L:208:THR:HG21	1.95	0.48
1:N:90:VAL:O	1:N:203:THR:HG23	2.13	0.48
1:O:137:LYS:HA	1:O:152:SER:HB3	1.95	0.48
1:M:112:LYS:HD3	1:M:164:THR:OG1	2.13	0.48
1:O:203:THR:HG21	3:O:309:HOH:O	2.12	0.48
1:D:96:ILE:CD1	1:D:103:TYR:CE2	2.97	0.48
1:K:60:LYS:HD3	1:M:158:PRO:CD	2.43	0.48
1:N:76:HIS:NE2	1:N:78:LYS:HE2	2.29	0.48
1:P:156:GLY:HA2	3:P:455:HOH:O	2.13	0.48
1:I:90:VAL:C	1:I:129:MET:CE	2.82	0.48
1:P:66:ILE:HA	1:P:76:HIS:O	2.14	0.48
1:E:74:ARG:NH2	1:E:212:ILE:HG21	2.22	0.48
1:B:90:VAL:O	1:B:203:THR:HG23	2.14	0.48
1:D:96:ILE:HD12	1:D:202:PRO:HD3	1.95	0.48
1:H:183:THR:HG22	1:H:188:SER:HA	1.96	0.48
1:K:91:ARG:HG3	1:K:129:MET:HE1	1.95	0.47
1:P:114:ARG:HB3	1:P:208:THR:HG21	1.96	0.47
1:B:115:ASP:HB2	1:B:208:THR:HG21	1.96	0.47
1:D:39:LEU:HD22	1:D:53:LEU:HD13	1.97	0.47
1:K:203:THR:HG21	3:K:428:HOH:O	2.14	0.47
1:K:115:ASP:HB2	1:K:208:THR:HG21	1.96	0.47
1:G:62:LYS:HB3	1:G:90:VAL:HG23	1.97	0.47
1:H:226:ILE:O	1:H:230:MET:HG3	2.14	0.47
1:O:59:PRO:O	1:O:62:LYS:HE3	2.14	0.47
1:D:96:ILE:CD1	1:D:202:PRO:HG3	2.43	0.47
1:P:132:LEU:CD2	1:P:205:GLY:HA3	2.45	0.47
1:B:231:ARG:CG	1:B:231:ARG:HH11	2.25	0.47
1:D:39:LEU:HD22	1:D:53:LEU:CD1	2.45	0.47
1:E:112:LYS:HB3	1:E:165:THR:HG23	1.96	0.47
1:D:237:VAL:CG2	1:D:238:GLN:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:HD2	1:A:115:ASP:OD2	2.15	0.46
1:F:158:PRO:HG2	1:I:60:LYS:HD3	1.98	0.46
1:M:115:ASP:HB2	1:M:208:THR:HG21	1.98	0.46
1:P:132:LEU:CD2	1:P:205:GLY:C	2.84	0.46
1:A:48:GLN:HE22	1:A:55:ARG:HH21	1.62	0.46
1:B:203:THR:HG21	3:B:413:HOH:O	2.16	0.46
1:C:38:ARG:NH2	1:C:218:GLY:O	2.47	0.46
1:H:131:ARG:HH12	2:H:301:IMD:HN3	1.63	0.46
1:M:227:GLU:HA	1:M:230:MET:HE3	1.96	0.46
1:D:62:LYS:HB3	1:D:90:VAL:HG23	1.96	0.46
1:K:65:TYR:CD1	1:K:79:GLY:HA2	2.51	0.46
1:G:66:ILE:HG23	1:G:75:VAL:HG13	1.97	0.46
1:H:112:LYS:HB2	1:H:112:LYS:HE3	1.63	0.46
1:A:219:GLN:NE2	1:A:219:GLN:H	2.13	0.46
1:D:38:ARG:HD2	1:D:218:GLY:O	2.16	0.46
1:P:96:ILE:HA	1:P:97:PRO:HD3	1.73	0.46
1:J:230:MET:C	1:J:231:ARG:CG	2.84	0.46
1:A:137:LYS:HE2	1:A:138:HIS:NE2	2.31	0.45
1:D:137:LYS:HB3	1:D:137:LYS:NZ	2.30	0.45
1:O:132:LEU:CD2	1:O:205:GLY:C	2.85	0.45
1:A:48:GLN:NE2	1:A:55:ARG:HH21	2.14	0.45
1:O:37:ARG:HG3	1:O:41:ARG:HE	1.81	0.45
1:P:35:LEU:HD13	1:P:218:GLY:C	2.37	0.45
1:B:35:LEU:O	1:B:39:LEU:HG	2.16	0.45
1:J:42:LEU:HD22	1:J:230:MET:HE1	1.97	0.45
1:O:231:ARG:O	1:O:232:GLU:OE1	2.35	0.45
1:A:112:LYS:HG3	1:A:112:LYS:O	2.16	0.45
1:B:34:GLU:O	1:B:37:ARG:HB3	2.17	0.45
1:F:91:ARG:N	1:F:129:MET:HE2	2.30	0.45
1:M:226:ILE:O	1:M:230:MET:HG3	2.16	0.45
1:E:62:LYS:HB3	1:E:90:VAL:HG23	1.99	0.45
1:F:206:LEU:HD22	1:F:211:GLU:HB3	1.99	0.45
1:G:232:GLU:OE1	1:G:233:TRP:CE2	2.69	0.45
1:I:62:LYS:HB3	1:I:90:VAL:HG23	1.98	0.45
1:O:70:GLN:OE1	1:O:74:ARG:NH2	2.49	0.45
1:B:231:ARG:CG	1:B:231:ARG:NH1	2.80	0.45
1:D:115:ASP:HB2	1:D:208:THR:HG21	1.99	0.45
1:F:62:LYS:HB3	1:F:90:VAL:HG23	1.99	0.45
1:I:140:TYR:HB3	1:I:193:PHE:CE2	2.52	0.45
1:A:58:SER:OG	1:A:60:LYS:HG3	2.17	0.44
1:A:74:ARG:HG2	1:A:76:HIS:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:GLN:H	1:K:33:GLN:CD	2.20	0.44
1:M:38:ARG:HD2	1:M:218:GLY:O	2.18	0.44
1:O:63:TYR:HB3	1:O:88:ALA:HB1	1.99	0.44
1:P:35:LEU:CD2	1:P:55:ARG:CG	2.93	0.44
1:D:96:ILE:HD11	1:D:202:PRO:CG	2.45	0.44
1:G:137:LYS:HG2	1:G:138:HIS:CD2	2.53	0.44
1:F:180:CYS:HB2	1:F:196:LEU:HD11	2.00	0.44
1:F:42:LEU:HD21	1:F:227:GLU:HG2	1.99	0.44
1:I:137:LYS:CG	3:I:422:HOH:O	2.37	0.44
1:I:65:TYR:CD1	1:I:79:GLY:HA2	2.53	0.44
1:A:90:VAL:O	1:A:203:THR:HG23	2.18	0.44
1:O:55:ARG:HG3	1:O:55:ARG:HH21	1.82	0.44
1:D:49:HIS:C	1:D:49:HIS:ND1	2.71	0.44
1:F:90:VAL:C	1:F:129:MET:HE2	2.38	0.44
1:G:226:ILE:O	1:G:230:MET:HG3	2.17	0.44
1:K:62:LYS:HB3	1:K:90:VAL:HG23	1.99	0.44
1:O:91:ARG:NH1	1:O:129:MET:SD	2.91	0.44
1:C:38:ARG:HD3	1:C:218:GLY:O	2.18	0.44
1:P:112:LYS:HD2	1:P:164:THR:OG1	2.18	0.44
1:A:220:GLN:HB2	1:A:221:PRO:HD2	2.00	0.43
1:O:90:VAL:O	1:O:203:THR:HG23	2.18	0.43
1:C:38:ARG:HH21	1:C:38:ARG:CB	2.30	0.43
1:M:227:GLU:HA	1:M:230:MET:CE	2.49	0.43
1:M:67:GLY:HA3	1:M:76:HIS:CE1	2.53	0.43
1:P:112:LYS:HD2	1:P:164:THR:HG1	1.84	0.43
1:A:117:TYR:HB2	1:A:207:GLN:HB3	2.00	0.43
1:D:90:VAL:O	1:D:203:THR:HG23	2.18	0.43
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.88	0.43
1:D:237:VAL:HG22	1:D:238:GLN:N	2.33	0.43
1:L:203:THR:HG21	3:L:379:HOH:O	2.19	0.43
1:A:131:ARG:HH22	2:A:901:IMD:HN3	1.65	0.43
1:B:183:THR:HG22	1:B:188:SER:HA	2.00	0.43
1:C:181:PHE:HB3	1:C:191:ILE:HD13	2.00	0.43
1:J:42:LEU:HD22	1:J:230:MET:CE	2.48	0.43
1:P:78:LYS:HB2	1:P:78:LYS:HE3	1.59	0.42
1:A:130:ASN:O	1:A:131:ARG:HG2	2.19	0.42
1:A:140:TYR:HB3	1:A:193:PHE:CE2	2.55	0.42
1:F:90:VAL:CA	1:F:129:MET:CE	2.98	0.42
1:A:115:ASP:HB2	1:A:208:THR:HG21	2.02	0.42
1:B:33:GLN:O	1:B:37:ARG:HB2	2.19	0.42
1:B:34:GLU:HA	1:B:37:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:TYR:C	1:J:231:ARG:H	2.23	0.42
1:H:90:VAL:O	1:H:203:THR:HG23	2.18	0.42
1:H:47:ASN:C	1:H:47:ASN:OD1	2.58	0.42
1:I:39:LEU:HD13	1:I:53:LEU:HD12	2.00	0.42
1:O:39:LEU:HB3	1:O:53:LEU:HD12	2.00	0.42
1:I:91:ARG:H	1:I:129:MET:HE3	1.82	0.42
1:J:105:PHE:CE1	1:J:171:CYS:HB3	2.54	0.42
1:C:168:VAL:HG11	1:C:223:LEU:HD13	2.00	0.42
1:E:115:ASP:HB2	1:E:208:THR:HG21	2.01	0.42
1:P:34:GLU:HG3	1:P:35:LEU:N	2.34	0.42
1:F:194:THR:HG23	1:F:195:ASP:OD2	2.20	0.42
1:N:137:LYS:HA	1:N:152:SER:HB3	2.02	0.42
1:F:38:ARG:HD2	1:F:218:GLY:O	2.20	0.42
1:B:91:ARG:HG3	1:B:129:MET:HE1	2.02	0.42
1:O:81:GLY:HA3	1:O:209:PRO:HD3	2.02	0.42
1:F:90:VAL:O	1:F:203:THR:HG23	2.20	0.41
1:K:226:ILE:O	1:K:230:MET:HG3	2.19	0.41
1:C:66:ILE:HG23	1:C:75:VAL:HG13	2.00	0.41
1:M:66:ILE:HG23	1:M:75:VAL:HG13	2.02	0.41
1:O:55:ARG:CG	1:O:55:ARG:HH21	2.33	0.41
1:K:81:GLY:HA2	1:K:207:GLN:O	2.20	0.41
1:O:115:ASP:HB2	1:O:208:THR:HG21	2.02	0.41
1:E:227:GLU:HB3	1:M:231:ARG:HD2	2.01	0.41
1:I:38:ARG:HD2	1:I:218:GLY:O	2.21	0.41
1:I:90:VAL:HA	1:I:129:MET:HE2	1.85	0.41
1:K:35:LEU:O	1:K:39:LEU:HG	2.20	0.41
1:I:62:LYS:HA	1:I:129:MET:CE	2.45	0.41
1:M:29:SER:N	1:M:30:PRO:HD3	2.30	0.41
1:E:90:VAL:O	1:E:203:THR:HG23	2.20	0.41
1:L:223:LEU:HA	1:L:223:LEU:HD12	1.87	0.41
1:L:40:GLN:C	1:L:40:GLN:CD	2.78	0.41
1:B:231:ARG:NH1	1:B:231:ARG:HG3	2.29	0.41
1:B:96:ILE:HA	1:B:97:PRO:HD3	1.96	0.41
1:F:89:SER:O	1:F:129:MET:HE3	2.20	0.41
1:C:176:ILE:CD1	1:C:233:TRP:CZ3	3.03	0.41
1:P:91:ARG:HG3	1:P:129:MET:HE2	2.02	0.41
1:E:105:PHE:CE1	1:E:171:CYS:HB3	2.56	0.40
1:H:33:GLN:CG	1:H:34:GLU:N	2.85	0.40
1:I:105:PHE:CE1	1:I:171:CYS:HB3	2.56	0.40
1:I:131:ARG:HH12	2:J:301:IMD:H4	1.85	0.40
1:K:105:PHE:CE1	1:K:171:CYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PRO:HG2	1:D:96:ILE:HG13	2.02	0.40
1:L:33:GLN:H	1:L:33:GLN:CD	2.25	0.40
1:C:121:GLY:HA3	1:C:140:TYR:O	2.21	0.40
1:D:96:ILE:HA	1:D:97:PRO:HD3	1.99	0.40
1:I:90:VAL:C	1:I:129:MET:HE3	2.41	0.40
1:G:58:SER:HA	1:G:59:PRO:HD2	1.97	0.40
1:J:38:ARG:NH1	1:J:38:ARG:HB3	2.36	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	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
1	B	205/210 (98%)	197 (96%)	8 (4%)	0	100	100
1	C	203/210 (97%)	199 (98%)	4 (2%)	0	100	100
1	D	208/210 (99%)	204 (98%)	4 (2%)	0	100	100
1	E	205/210 (98%)	202 (98%)	3 (2%)	0	100	100
1	F	205/210 (98%)	198 (97%)	7 (3%)	0	100	100
1	G	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
1	H	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
1	I	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
1	J	197/210 (94%)	192 (98%)	5 (2%)	0	100	100
1	K	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
1	L	203/210 (97%)	197 (97%)	6 (3%)	0	100	100
1	M	206/210 (98%)	200 (97%)	5 (2%)	1 (0%)	34	17
1	N	201/210 (96%)	197 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	200/210 (95%)	193 (96%)	7 (4%)	0	100	100
1	P	202/210 (96%)	195 (96%)	7 (4%)	0	100	100
All	All	3246/3360 (97%)	3164 (98%)	81 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	30	PRO

### 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	170/173 (98%)	168 (99%)	2 (1%)	78	71
1	B	171/173 (99%)	171 (100%)	0	100	100
1	C	168/173 (97%)	166 (99%)	2 (1%)	78	71
1	D	173/173 (100%)	172 (99%)	1 (1%)	90	88
1	E	170/173 (98%)	170 (100%)	0	100	100
1	F	170/173 (98%)	168 (99%)	2 (1%)	78	71
1	G	167/173 (96%)	167 (100%)	0	100	100
1	H	167/173 (96%)	166 (99%)	1 (1%)	90	88
1	I	170/173 (98%)	168 (99%)	2 (1%)	78	71
1	J	164/173 (95%)	160 (98%)	4 (2%)	57	41
1	K	167/173 (96%)	167 (100%)	0	100	100
1	L	169/173 (98%)	169 (100%)	0	100	100
1	M	171/173 (99%)	170 (99%)	1 (1%)	90	88
1	N	167/173 (96%)	167 (100%)	0	100	100
1	O	166/173 (96%)	166 (100%)	0	100	100
1	P	168/173 (97%)	166 (99%)	2 (1%)	78	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2698/2768 (98%)	2681 (99%)	17 (1%)	90	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	219	GLN
1	C	34	GLU
1	C	232	GLU
1	D	34	GLU
1	F	29	SER
1	F	33	GLN
1	H	131	ARG
1	I	32	GLU
1	I	112	LYS
1	J	33	GLN
1	J	34	GLU
1	J	37	ARG
1	J	41	ARG
1	M	33	GLN
1	P	131	ARG
1	P	208	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	48	GLN
1	A	219	GLN
1	B	80	HIS
1	B	130	ASN
1	C	76	HIS
1	F	130	ASN
1	G	33	GLN
1	G	48	GLN
1	G	148	HIS
1	I	48	GLN
1	J	130	ASN
1	J	148	HIS
1	N	130	ASN
1	N	138	HIS

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Mol	Chain	Res	Type
1	O	80	HIS
1	P	148	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	IMD	A	901	-	3,5,5	0.57	0	4,5,5	0.54	0
2	IMD	D	301	-	3,5,5	0.51	0	4,5,5	0.50	0
2	IMD	E	301	-	3,5,5	0.62	0	4,5,5	0.38	0
2	IMD	G	301	-	3,5,5	0.45	0	4,5,5	0.82	0
2	IMD	H	301	-	3,5,5	0.56	0	4,5,5	0.59	0
2	IMD	J	301	-	3,5,5	0.67	0	4,5,5	0.50	0
2	IMD	N	301	-	3,5,5	0.67	0	4,5,5	0.37	0
2	IMD	P	301	-	3,5,5	0.52	0	4,5,5	0.56	0

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
2	IMD	A	901	-	-	0/0/0/0	0/1/1/1
2	IMD	D	301	-	-	0/0/0/0	0/1/1/1
2	IMD	E	301	-	-	0/0/0/0	0/1/1/1
2	IMD	G	301	-	-	0/0/0/0	0/1/1/1
2	IMD	H	301	-	-	0/0/0/0	0/1/1/1
2	IMD	J	301	-	-	0/0/0/0	0/1/1/1
2	IMD	N	301	-	-	0/0/0/0	0/1/1/1
2	IMD	P	301	-	-	0/0/0/0	0/1/1/1

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	IMD	2	0
2	H	301	IMD	3	0
2	J	301	IMD	1	0
2	P	301	IMD	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	206/210 (98%)	-0.55	0 100 100	8, 13, 30, 51	0
1	B	207/210 (98%)	-0.35	3 (1%) 78 74	9, 16, 39, 90	0
1	C	205/210 (97%)	-0.46	3 (1%) 76 72	8, 15, 38, 68	0
1	D	210/210 (100%)	-0.45	4 (1%) 70 66	9, 16, 34, 61	0
1	E	207/210 (98%)	-0.38	2 (0%) 84 82	8, 14, 29, 62	0
1	F	207/210 (98%)	-0.40	1 (0%) 91 90	8, 16, 35, 62	0
1	G	203/210 (96%)	-0.50	1 (0%) 91 90	7, 15, 29, 53	0
1	H	203/210 (96%)	-0.45	2 (0%) 84 82	8, 15, 32, 66	0
1	I	206/210 (98%)	-0.54	1 (0%) 91 90	5, 12, 25, 52	0
1	J	199/210 (94%)	-0.35	1 (0%) 91 90	6, 14, 35, 68	0
1	K	203/210 (96%)	-0.50	2 (0%) 84 82	7, 14, 30, 61	0
1	L	205/210 (97%)	-0.27	0 100 100	14, 21, 37, 60	0
1	M	208/210 (99%)	-0.49	3 (1%) 78 74	7, 13, 31, 71	0
1	N	203/210 (96%)	-0.47	0 100 100	7, 15, 34, 61	0
1	O	202/210 (96%)	-0.27	4 (1%) 68 64	11, 19, 43, 76	0
1	P	204/210 (97%)	0.08	9 (4%) 38 32	11, 25, 46, 72	0
All	All	3278/3360 (97%)	-0.40	36 (1%) 82 80	5, 16, 37, 90	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	31	GLY	4.7
1	P	49	HIS	3.9
1	B	238	GLN	3.9
1	M	33	GLN	3.7
1	D	30	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	32	GLU	3.5
1	B	33	GLN	3.4
1	P	55	ARG	3.3
1	P	52	PRO	3.3
1	D	49	HIS	3.3
1	P	53	LEU	3.1
1	C	33	GLN	3.0
1	B	34	GLU	2.9
1	P	51	THR	2.9
1	K	33	GLN	2.9
1	O	33	GLN	2.7
1	D	31	GLY	2.6
1	C	233	TRP	2.6
1	H	33	GLN	2.6
1	O	34	GLU	2.5
1	C	235	ALA	2.4
1	P	80	HIS	2.4
1	M	60	LYS	2.4
1	G	80	HIS	2.3
1	I	32	GLU	2.3
1	H	37	ARG	2.3
1	E	33	GLN	2.3
1	F	235	ALA	2.2
1	O	55	ARG	2.2
1	M	31	GLY	2.2
1	P	35	LEU	2.1
1	P	126	GLY	2.1
1	E	65	TYR	2.1
1	J	37	ARG	2.1
1	D	29	SER	2.0
1	P	56	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	IMD	N	301	5/5	0.93	0.12	5.49	8,13,18,19	0
2	IMD	D	301	5/5	0.94	0.11	5.32	14,18,20,23	0
2	IMD	E	301	5/5	0.96	0.12	5.20	11,13,15,18	0
2	IMD	J	301	5/5	0.94	0.10	4.87	11,12,22,23	0
2	IMD	H	301	5/5	0.95	0.14	3.08	13,13,17,20	0
2	IMD	A	901	5/5	0.94	0.10	2.76	9,15,15,17	0
2	IMD	G	301	5/5	0.94	0.12	1.84	15,16,20,26	0
2	IMD	P	301	5/5	0.90	0.09	0.25	27,29,34,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.