

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

#### Oct 31, 2021 – 01:01 AM EDT

PDB ID	:	3GJX
Title	:	Crystal Structure of the Nuclear Export Complex CRM1-Snurportin1-RanG
		TP
Authors	:	Monecke, T.; Guettler, T.; Neumann, P.; Dickmanns, A.; Goerlich, D.; Ficner,
		R.
Deposited on	:	2009-03-09
Resolution	:	2.50  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 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	:	2.23.2
buster-report	:	1.1.7 (2018)
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)	:	2.23.2

## 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 2.50 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
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	Qualit	ty of chain		
1	В	365	44%	26%	5% •	25%
1	Е	365	43%	30%	·	24%
2	С	216	% 47%	28%	·	21%
2	F	216	53%	23%	·	21%
3	А	1073	<u>6%</u> 56%		36%	5% •



Mol	Chain	Length	Quality of	of chain		
2	р	1072	9%			_
3	D	1073	55%	37%	•	•



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## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25280 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	В	974	Total	С	Ν	0	$\mathbf{S}$	0	n	0
1	D	274	2222	1413	379	415	15	0	2	0
1	F	270	Total	С	Ν	0	S	0	8	0
		219	2303	1466	394	427	16	0	0	0

• Molecule 1 is a protein called Snurportin-1.

Chain	Residue	Modelled	Actual	Comment	Reference
В	-4	GLY	-	expression tag	UNP O95149
В	-3	PRO	-	expression tag	UNP O95149
В	-2	LEU	-	expression tag	UNP O95149
В	-1	GLY	-	expression tag	UNP O95149
В	0	SER	-	expression tag	UNP O95149
Е	-4	GLY	-	expression tag	UNP O95149
Е	-3	PRO	-	expression tag	UNP O95149
Е	-2	LEU	-	expression tag	UNP O95149
Е	-1	GLY	-	expression tag	UNP 095149

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called GTP-binding nuclear protein Ran.

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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	С	171	Total	С	Ν	0	$\mathbf{S}$	0	1	0
			1399	910	246	238	5	0		
2	F	171	Total	С	Ν	Ο	S	0	0	0
2 Г	1/1	1389	904	243	237	5	0	U	U	

expression tag

UNP 095149

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826



• Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	А	1041	Total 8456	C 5424	N 1421	O 1557	S 54	0	5	0
3	D	1041	Total 8483	C 5438	N 1427	0 1564	S 54	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP Q6P5F9
А	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Na 1 1	0	0
4	Е	1	Total Na 1 1	0	0

• Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	С	1	Total	С	Ν	Ο	Р	0	0
5	5 C	1	32	10	5	14	3	0	
5	Б	1	Total	С	Ν	Ο	Р	0	0
5 F	1	32	10	5	14	3	0	0	

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf
7	Ε	1	Total 1	Cl 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	134	Total O 134 134	0	0
8	С	58	$\begin{array}{cc} \text{Total} & \text{O} \\ 58 & 58 \end{array}$	0	0
8	А	258	Total O 258 258	0	0
8	Е	130	Total O 130 130	0	0
8	F	46	Total         O           46         46	0	0
8	D	333	Total O 333 333	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: Snurportin-1









#### V441 1445 K446 D447 L480 L480 M481 N482 Q483 Q483 Q486 G486 G486 G486 S490 W491 W491 M476 R515 F516 L517 V518 V566 4457 3458 I52 K52 I 544 M545 L569 654 1708 Q709 L710 G711 R712 L689 G689 V720 Y721 K722 1737 1738 H704 <mark>V777</mark> P778 P779 L780 L781 <mark>V792</mark> R796 E797 P798 Q770 M771 K810 L811 F838 E839 181 F973 R887 N888 V889 A890 K957 1958 8959 1960 1961 1963 1963 1963 1966 1966 1966 .939 .940 955 0891 931 D1029 T1030 S1031 D1032 L1033 H988 L989 1974 VAL PRO GLY TLE LEU ASN PRO GLU TLE PRO GLU GLU MET ASP



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	72.17Å $225.74$ Å $163.45$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $100.56^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	38.84 - 2.50	Depositor
Resolution (A)	47.81 - 2.50	EDS
% Data completeness	97.4 (38.84-2.50)	Depositor
(in resolution range)	86.9(47.81-2.50)	EDS
$R_{merge}$	0.12	Depositor
R <sub>sym</sub>	0.12	Depositor
$< I/\sigma(I) > 1$	$2.82 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
D D	0.244 , $0.281$	Depositor
$n, n_{free}$	0.246 , $0.282$	DCC
$R_{free}$ test set	8606 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $46.6$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.41, < L^2>=0.24$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	25280	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.14% 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: MG, NA, GTP, CL

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).

Mal	Chain	Chain Bond lengths		Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.42	0/2283	0.74	3/3090~(0.1%)	
1	Е	0.40	0/2364	0.64	0/3202	
2	С	0.34	0/1434	0.52	0/1936	
2	F	0.33	0/1423	0.56	2/1921~(0.1%)	
3	А	0.36	0/8628	0.51	0/11687	
3	D	0.36	0/8656	0.51	0/11724	
All	All	0.37	0/24788	0.55	5/33560~(0.0%)	

There are no bond length outliers.

All	(5)	bond	angle	outliers	are	listed	below:	
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	351	PRO	CA-N-CD	-10.95	96.18	111.50
1	В	352	ASP	N-CA-C	6.65	128.97	111.00
2	F	13	LEU	CA-CB-CG	5.79	128.61	115.30
1	В	215	GLU	N-CA-C	-5.18	97.00	111.00
2	F	13	LEU	CB-CG-CD1	5.02	119.54	111.00

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	В	2222	0	2151	107	0
1	Е	2303	0	2223	105	0
2	С	1399	0	1425	60	0
2	F	1389	0	1419	52	0
3	А	8456	0	8516	419	0
3	D	8483	0	8530	417	0
4	В	1	0	0	0	0
4	Ε	1	0	0	0	0
5	С	32	0	12	2	0
5	F	32	0	12	2	0
6	С	1	0	0	0	0
6	F	1	0	0	0	0
7	Ε	1	0	0	1	0
8	А	258	0	0	15	0
8	В	134	0	0	8	0
8	С	58	0	0	3	0
8	D	333	0	0	9	0
8	Е	130	0	0	7	0
8	F	46	0	0	2	0
All	All	25280	0	24288	1137	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 23.

All (1137) 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)
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.18	1.13
2:F:54:THR:HG22	2:F:176:PHE:HB3	1.19	1.11
3:D:33:ASN:HB2	3:D:44:ARG:HG3	1.33	1.09
3:A:1008:ILE:HG23	3:A:1009:PRO:HD3	1.35	1.07
1:E:350:SER:HB3	1:E:351:PRO:HD2	1.37	1.05
1:E:351:PRO:HB3	7:E:362:CL:CL	1.97	1.01
3:A:256:ASN:HB3	3:A:293:GLN:HE21	1.22	1.00
3:D:426:LYS:H	3:D:426:LYS:HD2	1.25	0.99
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.07	0.98
3:D:960:THR:HG23	3:D:968:VAL:HG11	1.41	0.98
3:D:1008:ILE:HG23	3:D:1009:PRO:HD3	1.42	0.97
3:A:33:ASN:HB2	3:A:44:ARG:HG3	1.47	0.97
3:A:426:LYS:H	3:A:426:LYS:HD2	1.28	0.96
3:A:962:LEU:HD23	3:A:968:VAL:HG21	1.44	0.95
3:D:434:GLU:HG3	3:D:440:VAL:HG12	1.46	0.95



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	• · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.31	0.95
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.09	0.94
3:A:1016:ARG:HG2	3:A:1016:ARG:HH11	1.30	0.94
3:D:46:ALA:O	3:D:50:LEU:HB2	1.66	0.94
3:D:62:ARG:HB3	3:D:66:ILE:HD11	1.51	0.93
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.34	0.92
3:A:807:ILE:HD11	3:A:815:ILE:HD12	1.50	0.92
2:C:21:THR:HG23	2:C:89:MET:HG2	1.48	0.92
3:A:144:LYS:HG3	3:A:145:HIS:CD2	2.05	0.91
1:B:159:GLY:O	1:B:160:ASN:HB2	1.69	0.91
3:D:53:LEU:HD12	3:D:54:LYS:H	1.35	0.91
3:D:340:ARG:HG2	3:D:342:ASN:OD1	1.71	0.91
3:A:141:GLU:HA	3:A:144:LYS:HE2	1.54	0.90
1:E:43:ARG:HD2	1:E:46:ARG:HH12	1.35	0.89
3:A:46:ALA:O	3:A:50:LEU:HB2	1.72	0.88
3:D:770:GLN:HB3	8:D:1380:HOH:O	1.72	0.88
3:D:79:GLY:O	3:D:82:ILE:HG22	1.74	0.88
1:E:52[A]:LYS:HE3	1:E:265:HIS:H	1.39	0.87
2:C:134:LYS:HE3	2:C:135:SER:OG	1.75	0.86
3:D:63:VAL:HA	3:D:76:LYS:HG2	1.54	0.86
3:A:62:ARG:HH11	3:A:79:GLY:HA2	1.41	0.86
3:A:740:THR:HA	3:A:745[B]:ILE:HD13	1.58	0.86
3:A:53:LEU:HD12	3:A:54:LYS:H	1.41	0.85
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.11	0.85
3:A:393:LEU:HD22	3:A:398:GLN:HA	1.55	0.85
3:A:990:GLN:H	3:A:993:GLN:HE21	1.24	0.85
2:C:29:ARG:HB3	2:C:157:PHE:CZ	2.12	0.84
3:A:62:ARG:NH1	3:A:79:GLY:HA2	1.93	0.84
3:D:476:MET:HE3	3:D:501:ILE:HA	1.59	0.84
1:B:52:LYS:HE3	1:B:264:THR:HA	1.57	0.84
1:E:43:ARG:HD2	1:E:46:ARG:NH1	1.92	0.83
3:A:451:ILE:HG12	8:A:1203:HOH:O	1.78	0.82
3:D:393:LEU:HD12	3:D:395:SER:H	1.44	0.82
3:D:990:GLN:H	3:D:993:GLN:HE21	1.27	0.82
1:B:285:VAL:HG12	1:B:286:LEU:HD12	1.62	0.82
1:E:200:GLN:HG2	8:E:497:HOH:O	1.80	0.80
1:B:38:LEU:HG	1:B:40:GLN:H	1.46	0.80
3:A:1048:GLU:HG3	3:A:1052:LEU:HG	1.63	0.80
3:A:30:ASN:ND2	3:A:47:GLN:HE22	1.80	0.79
1:B:156:LEU:HD13	1:B:218:LEU:HD11	1.65	0.79
3:A:94:LEU:HD23	3:A:95:PRO:HD2	1.65	0.79



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Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:426:LYS:H	3:D:426:LYS:CD	1.94	0.79
3:D:476:MET:CE	3:D:501:ILE:HG12	2.12	0.79
3:A:276:VAL:HG21	3:A:336:LEU:HD22	1.64	0.79
1:B:264:THR:HG22	1:B:265:HIS:O	1.84	0.78
3:D:23:LEU:HD23	3:D:26:ASN:HB2	1.66	0.78
3:D:276:VAL:HG21	3:D:336:LEU:HD22	1.65	0.78
1:B:108:LEU:HB3	1:B:277:LEU:HD13	1.66	0.78
3:A:214:GLU:HG3	3:A:215:ASN:ND2	2.00	0.77
3:A:962:LEU:HB2	3:A:973:PHE:CD2	2.19	0.77
3:A:509[B]:HIS:HD2	3:A:511:GLU:H	1.33	0.77
3:A:107:VAL:O	3:A:111:ILE:HG12	1.85	0.77
3:D:214:GLU:HG3	3:D:215:ASN:ND2	2.00	0.77
3:D:781:LEU:HD11	3:D:821:GLN:HG3	1.67	0.77
3:D:962:LEU:HB2	3:D:973:PHE:CD2	2.20	0.76
3:A:32:VAL:HG22	3:A:71:GLN:HG2	1.66	0.76
1:E:38:LEU:HG	1:E:40:GLN:H	1.48	0.76
3:A:990:GLN:HG3	3:A:993:GLN:HG3	1.68	0.76
1:B:102:LEU:HD13	1:B:129:ARG:HH11	1.51	0.76
3:A:289:LEU:O	3:A:292:MET:HG3	1.84	0.76
3:A:426:LYS:H	3:A:426:LYS:CD	1.98	0.76
3:A:476:MET:HE3	3:A:501:ILE:CG1	2.09	0.76
3:D:990:GLN:HG3	3:D:993:GLN:HG3	1.68	0.75
1:B:359:GLU:HG2	8:B:494:HOH:O	1.84	0.75
3:D:392:PRO:HA	3:D:399:HIS:NE2	2.02	0.75
3:A:704:HIS:CD2	3:A:767[B]:ASN:H	2.05	0.74
1:B:102:LEU:HB3	1:B:129:ARG:NH1	2.02	0.74
3:A:55:GLU:HG2	3:A:56:HIS:H	1.52	0.74
2:F:54:THR:CG2	2:F:176:PHE:HB3	2.10	0.74
3:A:476:MET:HE2	3:A:516:PHE:HZ	1.52	0.73
3:D:53:LEU:HD12	3:D:54:LYS:N	2.02	0.73
3:A:476:MET:HE2	3:A:516:PHE:CZ	2.24	0.73
3:D:56:HIS:CG	3:D:56:HIS:O	2.41	0.73
3:D:1033:LEU:HD12	3:D:1035:LEU:HD11	1.71	0.73
3:A:56:HIS:CG	3:A:56:HIS:O	2.42	0.72
3:A:116:ASP:O	3:A:119:CYS:HB3	1.90	0.72
2:C:95:ARG:HD2	2:C:130:LYS:HB3	1.71	0.72
3:A:888:ASN:ND2	3:A:889:VAL:H	1.88	0.72
3:D:341:LEU:HD23	3:D:344:ARG:HD2	1.70	0.72
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.24	0.72
3:A:97:ASN:H	3:A:97:ASN:ND2	1.87	0.72
3:D:678:ILE:HD12	3:D:679:LEU:H	1.55	0.72



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:509[B]:HIS:CD2	3:A:511:GLU:HB3	2.24	0.71
3:A:665:TRP:O	3:A:669:ILE:HG12	1.88	0.71
3:A:509[B]:HIS:CD2	3:A:511:GLU:H	2.07	0.71
3:A:704:HIS:CD2	3:A:767[A]:ASN:H	2.09	0.71
3:D:738:MET:HG3	8:D:1269:HOH:O	1.90	0.71
3:A:739:VAL:O	3:A:745[B]:ILE:HG21	1.90	0.71
3:D:32:VAL:O	3:D:36:TYR:HD2	1.72	0.71
3:D:434:GLU:HG3	3:D:440:VAL:CG1	2.19	0.71
3:A:20:SER:HB2	3:A:22:LYS:HG3	1.72	0.71
3:D:144:LYS:HG3	3:D:145[A]:HIS:CD2	2.26	0.71
3:A:32:VAL:O	3:A:36:TYR:HD2	1.73	0.70
3:D:888:ASN:ND2	3:D:889:VAL:H	1.89	0.70
3:A:1043:ARG:NH1	3:A:1046:GLN:HG2	2.06	0.70
3:A:249:THR:O	3:A:253:LYS:HB2	1.90	0.70
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.71	0.70
3:D:672:ALA:HA	3:D:678:ILE:HD11	1.72	0.70
2:C:21:THR:HG22	2:C:23:LYS:HG3	1.72	0.70
3:D:312:LYS:HE3	3:D:312:LYS:HA	1.73	0.70
3:A:179:PHE:CE1	3:A:195:LYS:HG2	2.25	0.70
3:D:28:LEU:HD11	3:D:66:ILE:HG23	1.73	0.70
3:D:131:ASN:ND2	3:D:166:ASN:HD21	1.85	0.70
3:A:672:ALA:HA	3:A:678:ILE:HD11	1.72	0.70
3:D:249:THR:O	3:D:253:LYS:HB2	1.90	0.69
3:D:665:TRP:O	3:D:669:ILE:HG12	1.90	0.69
3:D:179:PHE:HE1	3:D:195:LYS:HE2	1.58	0.69
3:A:71:GLN:HA	3:A:74:ASN:OD1	1.92	0.69
3:A:226:LEU:HD23	3:A:263:VAL:HB	1.75	0.69
3:D:58:ASP:OD1	3:D:61:THR:HB	1.92	0.69
1:E:70:TRP:CE3	1:E:96:LYS:O	2.45	0.69
1:B:159:GLY:O	1:B:160:ASN:CB	2.40	0.69
3:A:803:THR:O	3:A:807:ILE:HG23	1.92	0.69
3:D:957:LYS:NZ	3:D:961:PRO:HB3	2.07	0.69
2:C:70:GLU:O	2:C:76:ARG:NH2	2.26	0.69
3:A:53:LEU:HD12	3:A:54:LYS:N	2.06	0.69
3:D:141:GLU:HA	3:D:144:LYS:HE2	1.75	0.69
3:D:704:HIS:CD2	3:D:767:ASN:H	2.11	0.69
2:C:169:ILE:HG22	2:C:170:GLY:H	1.58	0.68
3:D:424:MET:HA	3:D:457:MET:HE2	1.76	0.68
3:A:957:LYS:NZ	3:A:961:PRO:HB3	2.07	0.68
3:D:962:LEU:C	3:D:964:PRO:HD3	2.13	0.68
3:A:179:PHE:HE1	3:A:195:LYS:HE2	1.59	0.68



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:300:LEU:O	3:A:352:HIS:HE1	1.76	0.68
3:A:205:ILE:HD11	3:A:232:PHE:CZ	2.28	0.68
3:A:1016:ARG:HG2	3:A:1016:ARG:NH1	1.98	0.68
3:D:97:ASN:H	3:D:97:ASN:ND2	1.89	0.68
3:D:737[A]:GLU:O	3:D:740:THR:HB	1.93	0.68
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.76	0.68
3:A:399:HIS:HD2	3:A:401:ASP:HB2	1.58	0.68
3:A:704:HIS:HD2	3:A:767[B]:ASN:H	1.38	0.68
3:A:737:GLU:O	3:A:740:THR:HB	1.94	0.68
1:B:261:HIS:HD2	1:B:263:GLN:H	1.40	0.68
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.76	0.68
1:E:105:SER:HA	1:E:274:VAL:HG13	1.76	0.68
3:A:28:LEU:O	3:A:32:VAL:HG23	1.94	0.68
3:D:300:LEU:O	3:D:352:HIS:HE1	1.77	0.67
3:A:815:ILE:HG12	3:A:818:GLU:HG2	1.76	0.67
2:C:38:LYS:HG2	3:A:842:PRO:HG3	1.76	0.67
1:E:43:ARG:CD	1:E:46:ARG:HH12	2.07	0.67
1:E:123:VAL:HG21	1:E:250:PHE:CZ	2.29	0.67
3:D:251:ILE:HG21	3:D:289:LEU:HB3	1.76	0.67
3:A:962:LEU:HD13	3:A:973:PHE:HE2	1.60	0.67
3:D:226:LEU:HD23	3:D:263:VAL:HB	1.76	0.67
3:D:1043:ARG:NH1	3:D:1046:GLN:HG2	2.09	0.67
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.67
3:D:815:ILE:HG12	3:D:818:GLU:HG2	1.77	0.67
2:F:106:ARG:HD3	3:D:181:PHE:CE2	2.30	0.67
1:B:222:THR:HG22	1:B:225:ASN:H	1.59	0.67
2:C:21:THR:CG2	2:C:89:MET:HG2	2.24	0.67
3:A:131:ASN:ND2	3:A:166:ASN:HD21	1.87	0.67
1:E:52[A]:LYS:CE	1:E:265:HIS:H	2.08	0.66
3:D:179:PHE:CE1	3:D:195:LYS:HG2	2.29	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.09	0.66
1:B:176:TYR:HB2	1:B:183:TYR:CE1	2.29	0.66
3:A:63:VAL:HA	3:A:76:LYS:HG2	1.76	0.66
3:D:482:ASN:HB3	3:D:488:GLU:HB2	1.76	0.66
3:D:737[B]:GLU:O	3:D:740:THR:HB	1.94	0.66
1:E:176:TYR:HB2	1:E:183:TYR:CE1	2.29	0.66
2:C:37:LYS:HE3	8:A:1199:HOH:O	1.96	0.66
1:E:207:TRP:HB3	8:E:492:HOH:O	1.95	0.66
1:E:160:ASN:O	1:E:161:ARG:HG2	1.96	0.66
3:D:435:ASN:ND2	3:D:439:GLU:HB2	2.09	0.66
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.78	0.66



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:482:ASN:HB3	3:A:488:GLU:HB2	1.77	0.66
3:A:388:THR:HG22	3:A:399:HIS:HE2	1.61	0.66
3:D:434:GLU:CG	3:D:440:VAL:HG12	2.25	0.66
1:B:160:ASN:CG	1:B:161:ARG:H	1.99	0.66
3:D:206:PHE:CE1	3:D:240:TYR:HB3	2.31	0.66
3:D:548:VAL:HG13	3:D:555:LEU:HD21	1.78	0.66
3:D:926:ILE:HG21	3:D:946:LEU:HD11	1.77	0.66
3:A:962:LEU:HD22	3:A:968:VAL:HG11	1.77	0.65
3:D:202:PHE:O	3:D:205:ILE:HG12	1.96	0.65
1:B:4:LEU:HD11	3:A:521:ILE:HG13	1.78	0.65
3:A:887:ARG:HH21	3:A:891:ASP:HB3	1.61	0.65
3:A:729:SER:OG	3:A:792:VAL:HG22	1.97	0.65
3:D:28:LEU:O	3:D:32:VAL:HG23	1.96	0.65
2:C:55:ASN:OD1	2:C:174:LEU:HD12	1.97	0.65
3:A:424:MET:HA	3:A:457:MET:HE2	1.79	0.65
1:E:127:GLY:HA2	8:E:549:HOH:O	1.97	0.65
3:D:33:ASN:HB2	3:D:44:ARG:CG	2.18	0.65
1:E:95:PRO:HB2	1:E:101:GLN:NE2	2.12	0.65
3:A:171:LEU:HD13	3:A:205:ILE:HD12	1.79	0.65
2:C:106:ARG:HD3	3:A:181:PHE:CE2	2.32	0.64
3:D:489:TRP:O	3:D:490:SER:HB3	1.97	0.64
3:A:704:HIS:HD2	3:A:767[A]:ASN:H	1.42	0.64
1:B:18:LEU:HA	1:B:36:SER:O	1.97	0.64
3:A:62:ARG:HH12	3:A:82:ILE:HG13	1.63	0.64
1:E:261:HIS:HD2	1:E:263:GLN:H	1.44	0.64
3:D:52:HIS:ND1	3:D:82:ILE:HD12	2.12	0.64
3:D:201:GLU:O	3:D:204:GLN:HG3	1.97	0.64
3:A:437:GLN:HG2	3:A:746:ARG:HG2	1.79	0.64
1:E:4:LEU:HD11	3:D:521:ILE:HG13	1.78	0.64
3:A:678:ILE:HD12	3:A:679:LEU:N	2.12	0.64
1:B:123:VAL:HG21	1:B:250:PHE:CZ	2.33	0.64
3:D:210:GLN:O	3:D:214:GLU:HG2	1.97	0.64
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.33	0.63
3:D:887:ARG:HH21	3:D:891:ASP:HB3	1.63	0.63
3:A:548:VAL:HG13	3:A:555:LEU:HD21	1.80	0.63
3:A:677:ASP:O	3:A:680:LYS:HB3	1.98	0.63
3:D:677:ASP:O	3:D:680:LYS:HB3	1.98	0.63
3:A:30:ASN:HD22	3:A:47:GLN:HE22	1.45	0.63
3:D:257:VAL:HG21	3:D:260:PHE:HD2	1.63	0.63
3:A:489:TRP:O	3:A:490:SER:HB3	1.98	0.63
3:A:257:VAL:HG21	3:A:260:PHE:HD2	1.64	0.63



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:678:ILE:HD12	3:A:679:LEU:H	1.64	0.63
3:A:926:ILE:HG21	3:A:946:LEU:HD11	1.80	0.63
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.34	0.63
3:D:704:HIS:HD2	3:D:767:ASN:H	1.45	0.63
3:A:678:ILE:C	3:A:680:LYS:H	2.02	0.63
3:D:22:LYS:HG2	3:D:58:ASP:CG	2.19	0.63
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.34	0.63
3:D:276:VAL:HA	3:D:283:PHE:CE2	2.34	0.63
3:D:678:ILE:C	3:D:680:LYS:H	2.02	0.63
1:B:102:LEU:HB3	1:B:129:ARG:HH12	1.64	0.62
3:A:888:ASN:HD22	3:A:889:VAL:H	1.46	0.62
3:A:961:PRO:HD3	3:A:970:ASN:HD21	1.62	0.62
1:E:18:LEU:HA	1:E:36:SER:O	1.99	0.62
3:A:229:LEU:HD11	3:A:246:LEU:HD11	1.80	0.62
3:A:388:THR:HG23	3:A:401:ASP:HB3	1.81	0.62
3:D:45:MET:O	3:D:49:VAL:HG12	1.98	0.62
3:A:187:THR:HG22	3:A:190:LYS:HB2	1.81	0.62
2:C:42:THR:HG23	8:C:826:HOH:O	1.98	0.62
3:A:276:VAL:HA	3:A:283:PHE:CE2	2.35	0.62
3:A:583:MET:HG2	8:A:1255:HOH:O	1.98	0.62
3:A:681:ASP:OD2	3:A:684:THR:HG23	2.00	0.62
3:A:810:LYS:O	3:A:810:LYS:HD3	1.99	0.62
3:D:437:GLN:HG2	3:D:746:ARG:HG2	1.81	0.62
3:A:1046:GLN:O	3:A:1049:LYS:HB2	1.99	0.62
1:E:278:ARG:HG2	1:E:281:MET:HE3	1.82	0.62
3:D:429:GLU:HG3	3:D:445:MET:HG3	1.82	0.62
3:D:476:MET:CE	3:D:516:PHE:HZ	2.13	0.62
3:D:90:ARG:O	3:D:94:LEU:HG	1.99	0.62
3:D:485:ASN:C	3:D:487:THR:H	2.04	0.62
3:D:229:LEU:HD11	3:D:246:LEU:HD11	1.81	0.61
3:D:476:MET:HE2	3:D:501:ILE:HG12	1.80	0.61
1:B:-1:GLY:O	1:B:3:GLU:HG2	1.99	0.61
3:A:216:SER:O	3:A:217:GLN:HG2	1.98	0.61
3:A:476:MET:CE	3:A:501:ILE:HG12	2.12	0.61
3:A:187:THR:HG22	3:A:190:LYS:HE3	1.81	0.61
3:D:32:VAL:HG22	3:D:71:GLN:HB2	1.82	0.61
1:B:285:VAL:HG12	1:B:286:LEU:CD1	2.29	0.61
3:A:210:GLN:O	3:A:214:GLU:HG2	1.99	0.61
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.28	0.61
3:A:110:ILE:CD1	3:A:130:LEU:HB3	2.30	0.61
3:D:141:GLU:HG2	3:D:145[A]:HIS:HD2	1.63	0.61



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:50:LEU:HD12	2:C:63:VAL:HG21	1.82	0.61
3:A:1003:SER:HA	3:A:1046:GLN:NE2	2.15	0.61
1:B:261:HIS:CD2	1:B:263:GLN:H	2.19	0.61
3:A:30:ASN:HA	3:A:44:ARG:HD2	1.82	0.61
3:D:888:ASN:HD22	3:D:889:VAL:H	1.46	0.61
3:D:28:LEU:CD1	3:D:66:ILE:HG23	2.29	0.61
3:D:544:ILE:HG22	3:D:545:MET:HE1	1.83	0.61
1:B:160:ASN:CG	1:B:161:ARG:N	2.54	0.61
1:E:52[A]:LYS:HE3	1:E:265:HIS:N	2.12	0.61
2:F:54:THR:HA	2:F:176:PHE:HA	1.83	0.61
3:A:62:ARG:NH1	3:A:82:ILE:HG13	2.15	0.60
3:D:402:ILE:HD13	3:D:407:GLN:NE2	2.16	0.60
3:D:1050:HIS:O	3:D:1054:MET:HG2	2.01	0.60
1:B:211:LYS:HD2	1:B:211:LYS:N	2.16	0.60
3:A:485:ASN:C	3:A:487:THR:H	2.05	0.60
1:B:218:LEU:HG	1:B:229:PHE:HB2	1.83	0.60
3:A:131:ASN:HD21	3:A:166:ASN:ND2	1.91	0.60
3:A:962:LEU:C	3:A:964:PRO:HD3	2.22	0.60
3:D:218:ASN:HD22	3:D:220:PRO:HD2	1.67	0.60
3:A:45:MET:O	3:A:49:VAL:HG12	2.00	0.60
3:A:962:LEU:O	3:A:963:ASN:HB2	2.01	0.60
2:F:117:ILE:HB	2:F:144:LEU:HD22	1.84	0.60
3:A:33:ASN:HB2	3:A:44:ARG:CG	2.26	0.60
3:A:225:THR:O	3:A:228:THR:HG22	2.02	0.60
3:A:295:LYS:HG2	3:A:300:LEU:HD11	1.83	0.60
3:D:429:GLU:HB3	3:D:445:MET:HB2	1.84	0.60
1:E:264:THR:HB	1:E:273:LEU:HD13	1.84	0.60
2:F:10:GLN:HG2	2:F:60:LYS:HD3	1.83	0.60
3:D:225:THR:O	3:D:228:THR:HG22	2.01	0.60
2:F:54:THR:HG22	2:F:176:PHE:CB	2.13	0.59
3:D:22:LYS:HG2	3:D:58:ASP:OD1	2.02	0.59
3:D:300:LEU:HD12	3:D:300:LEU:H	1.66	0.59
1:E:261:HIS:CD2	1:E:263:GLN:H	2.20	0.59
3:A:32:VAL:HG22	3:A:71:GLN:CG	2.32	0.59
2:F:50:LEU:HD12	2:F:63:VAL:HG21	1.84	0.59
1:E:211:LYS:HD2	1:E:211:LYS:N	2.18	0.59
3:A:206:PHE:HE2	3:A:244:THR:HG21	1.66	0.59
3:A:216:SER:HB2	3:A:222:VAL:CG2	2.33	0.59
1:E:128:LYS:O	1:E:175:ILE:HA	2.03	0.59
3:A:33:ASN:ND2	3:A:44:ARG:HE	1.99	0.59
3:D:218:ASN:ND2	3:D:220:PRO:HD2	2.18	0.59



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:295:LYS:HG2	3:D:300:LEU:HD11	1.84	0.59
3:A:483:GLN:HE22	3:A:489:TRP:HA	1.68	0.59
1:B:52:LYS:CE	1:B:265:HIS:H	2.15	0.59
1:B:52:LYS:HD3	1:B:265:HIS:CG	2.37	0.59
3:A:728:ILE:HD13	3:A:749:ARG:HD2	1.85	0.59
1:B:201:THR:HG22	1:B:264:THR:O	2.03	0.58
3:A:429:GLU:HG3	3:A:445:MET:HG3	1.85	0.58
3:A:476:MET:CE	3:A:516:PHE:HZ	2.15	0.58
3:D:681:ASP:OD2	3:D:684:THR:HG23	2.03	0.58
3:A:218:ASN:HD22	3:A:220:PRO:HD2	1.68	0.58
3:A:300:LEU:H	3:A:300:LEU:HD12	1.67	0.58
3:A:838:PHE:HA	3:A:845:ARG:NH2	2.18	0.58
3:D:476:MET:HE1	3:D:516:PHE:CZ	2.38	0.58
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.38	0.58
2:C:177:VAL:O	2:C:178:ALA:HB3	2.04	0.58
3:A:30:ASN:ND2	3:A:47:GLN:NE2	2.49	0.58
1:E:209:HIS:CE1	1:E:232:LEU:O	2.57	0.58
3:D:216:SER:HB2	3:D:222:VAL:CG2	2.34	0.58
3:D:293:GLN:O	3:D:297:MET:HG3	2.02	0.58
3:D:483:GLN:HE22	3:D:489:TRP:HA	1.69	0.58
3:D:926:ILE:HG21	3:D:946:LEU:CD1	2.34	0.58
3:A:265:LEU:HD21	3:A:322:LEU:HA	1.84	0.58
1:E:52[B]:LYS:NZ	1:E:263:GLN:O	2.34	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.18	0.58
2:C:117:ILE:HB	2:C:144:LEU:HD22	1.86	0.58
3:A:745[A]:ILE:HD13	3:A:748:MET:CE	2.33	0.58
1:E:185:VAL:HG12	1:E:208:MET:SD	2.44	0.58
3:D:146:TRP:N	3:D:147:PRO:HD3	2.18	0.58
2:F:52:PHE:HB2	2:F:59:ILE:HG22	1.86	0.58
3:D:62:ARG:O	3:D:66:ILE:HG13	2.04	0.58
3:D:340:ARG:HB3	3:D:343:LEU:HD12	1.85	0.57
3:D:545:MET:HG3	3:D:583:MET:SD	2.43	0.57
1:B:128:LYS:HE3	1:B:176:TYR:HD2	1.69	0.57
1:E:259:PHE:O	1:E:274:VAL:HA	2.03	0.57
3:D:150:ILE:HD11	3:D:205:ILE:HG23	1.85	0.57
3:D:360:VAL:HG11	3:D:365:ILE:HD12	1.85	0.57
3:D:597:ARG:HE	3:D:601:GLN:NE2	2.02	0.57
3:A:218:ASN:ND2	3:A:220:PRO:HD2	2.20	0.57
1:E:173:ASP:HB2	1:E:189:MET:HE1	1.85	0.57
3:D:92:LYS:HD2	3:D:1030:THR:HG21	1.86	0.57
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.24	0.57



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:52:PHE:HB2	2:C:59:ILE:HG22	1.86	0.57
3:A:146:TRP:N	3:A:147:PRO:HD3	2.18	0.57
3:A:399:HIS:CD2	3:A:401:ASP:HB2	2.40	0.57
3:A:705:PRO:O	3:A:708:ILE:HG22	2.04	0.57
3:A:799:GLU:HG2	8:A:1286:HOH:O	2.04	0.57
3:A:962:LEU:O	3:A:964:PRO:HD3	2.03	0.57
3:D:485:ASN:O	3:D:487:THR:N	2.38	0.57
3:D:1005:ASN:OD1	3:D:1049:LYS:HE3	2.05	0.57
3:A:303:ASN:HD21	3:A:305:ARG:NH2	2.03	0.57
3:D:728:ILE:HD13	3:D:749:ARG:HD2	1.87	0.57
1:B:259:PHE:O	1:B:274:VAL:HA	2.05	0.57
3:A:160:SER:HB3	3:A:163:LEU:HD12	1.87	0.57
3:A:341:LEU:HD23	3:A:341:LEU:O	2.05	0.57
3:D:107:VAL:O	3:D:111:ILE:HG12	2.05	0.57
3:A:388:THR:HG23	3:A:401:ASP:CB	2.35	0.57
1:E:26:PRO:HG2	1:E:109:ILE:HD11	1.87	0.57
3:D:21:GLN:HG2	3:D:22:LYS:N	2.20	0.57
3:D:265:LEU:HD21	3:D:322:LEU:HA	1.86	0.57
3:D:1038:ARG:HH21	3:D:1042:LEU:HD21	1.69	0.57
2:F:123:LYS:HE2	5:F:217:GTP:C4	2.40	0.56
3:D:810:LYS:O	3:D:810:LYS:HD3	2.05	0.56
1:B:278:ARG:HG2	1:B:281:MET:HE3	1.87	0.56
3:A:441:VAL:HB	3:A:628:GLN:OE1	2.05	0.56
3:A:681:ASP:O	3:A:685:VAL:HG13	2.05	0.56
2:F:9:VAL:O	2:F:9:VAL:HG22	2.04	0.56
3:D:91:TRP:HA	3:D:94:LEU:HD12	1.88	0.56
2:C:31:LEU:HD12	2:C:32:THR:CG2	2.36	0.56
3:A:344:ARG:NH1	3:A:408:LEU:HD21	2.21	0.56
3:A:961:PRO:HD3	3:A:970:ASN:ND2	2.21	0.56
3:D:851:LEU:O	3:D:855:VAL:HG23	2.06	0.56
3:A:481:GLN:OE1	3:A:481:GLN:HA	2.04	0.56
1:E:52[A]:LYS:HZ2	1:E:265:HIS:HB2	1.70	0.56
1:B:52:LYS:HE3	1:B:265:HIS:H	1.71	0.56
1:B:351:PRO:HB3	1:B:352:ASP:OD2	2.06	0.56
2:C:31:LEU:HD12	2:C:32:THR:HG23	1.88	0.56
3:A:150:ILE:HD11	3:A:205:ILE:HG22	1.86	0.56
3:A:926:ILE:HG21	3:A:946:LEU:CD1	2.36	0.56
3:D:142:TRP:HH2	3:D:198:MET:HA	1.71	0.56
1:B:209:HIS:CE1	1:B:232:LEU:O	2.58	0.56
3:A:360:VAL:HG11	3:A:365:ILE:HD12	1.86	0.56
3:D:84:GLU:O	3:D:88:LYS:HG3	2.05	0.56



9	0	$\mathbf{IV}$
0	G	JA

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:426:LYS:HD2	3:D:426:LYS:N	2.08	0.56
3:D:431:LEU:HD22	3:D:445:MET:CE	2.36	0.56
3:D:709:GLN:O	3:D:712:ARG:HB3	2.06	0.56
3:D:888:ASN:HD22	3:D:888:ASN:N	2.01	0.56
3:A:256:ASN:HB3	3:A:293:GLN:NE2	2.07	0.56
3:A:340:ARG:HB2	3:A:343:LEU:HD12	1.86	0.56
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.68	0.56
3:D:21:GLN:HG2	3:D:22:LYS:H	1.71	0.56
3:A:142:TRP:HH2	3:A:198:MET:HA	1.71	0.56
3:A:841:TYR:O	3:A:845:ARG:HG3	2.05	0.56
1:B:212:LEU:HB2	1:B:213:PRO:HD3	1.88	0.56
3:A:485:ASN:O	3:A:487:THR:N	2.39	0.56
3:A:957:LYS:HZ1	3:A:961:PRO:HB3	1.71	0.56
1:E:19:ASN:HD21	1:E:38:LEU:H	1.53	0.56
3:D:93:ILE:HG22	3:D:1027:GLY:HA3	1.88	0.56
3:D:312:LYS:HG3	3:D:313:ASP:H	1.70	0.56
2:C:10:GLN:HG2	2:C:60:LYS:HE2	1.87	0.55
1:B:61:HIS:HE1	1:B:101:GLN:HE22	1.53	0.55
1:E:52[A]:LYS:HE3	1:E:264:THR:HA	1.88	0.55
3:D:66:ILE:HG22	3:D:72:ASN:HB3	1.87	0.55
3:D:187:THR:HG23	3:D:190:LYS:H	1.72	0.55
3:D:962:LEU:HB2	3:D:973:PHE:HD2	1.68	0.55
3:D:1003:SER:HA	3:D:1046:GLN:NE2	2.21	0.55
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.26	0.55
3:A:388:THR:HG22	3:A:389:SER:N	2.21	0.55
3:D:132:MET:O	3:D:136:GLN:HG2	2.06	0.55
3:D:399:HIS:C	3:D:401:ASP:H	2.09	0.55
1:B:137:GLY:O	1:B:160:ASN:HB2	2.07	0.55
3:A:23:LEU:HD12	3:A:23:LEU:H	1.71	0.55
3:A:218:ASN:HB3	3:A:221:LEU:HB3	1.87	0.55
2:F:71:LYS:HG3	8:F:915:HOH:O	2.05	0.55
3:A:709:GLN:O	3:A:712:ARG:HB3	2.06	0.55
3:A:1016:ARG:HH11	3:A:1016:ARG:CG	2.13	0.55
3:A:293:GLN:O	3:A:297:MET:HG3	2.06	0.55
1:B:26:PRO:HG2	1:B:109:ILE:HD11	1.89	0.55
1:B:201:THR:HG22	1:B:204:ARG:NH1	2.21	0.55
3:A:514:LYS:NZ	8:A:1321:HOH:O	2.39	0.55
3:D:681:ASP:O	3:D:685:VAL:HG13	2.06	0.55
3:D:957:LYS:HZ1	3:D:961:PRO:HB3	1.71	0.55
3:D:960:THR:HG23	3:D:968:VAL:CG1	2.28	0.55
1:B:34:LYS:N	8:B:363:HOH:O	2.39	0.55



9	0	$\mathbf{IV}$
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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:360:ASN:HB2	8:B:494:HOH:O	2.06	0.55
1:E:349:HIS:CE1	3:D:708[A]:ILE:HD12	2.42	0.55
1:B:19:ASN:HD21	1:B:38:LEU:H	1.54	0.55
1:E:218:LEU:HG	1:E:229:PHE:HB2	1.89	0.55
2:F:155:TYR:HB2	3:D:445:MET:HE1	1.88	0.55
3:D:66:ILE:HG21	3:D:75:THR:HB	1.89	0.55
1:B:264:THR:OG1	1:B:273:LEU:HD13	2.07	0.54
3:A:132:MET:O	3:A:136:GLN:HG2	2.06	0.54
3:A:888:ASN:ND2	3:A:889:VAL:N	2.55	0.54
3:A:239:GLY:HA2	3:A:243:GLU:HG3	1.88	0.54
3:D:402:ILE:HG21	3:D:407:GLN:HE21	1.72	0.54
3:D:888:ASN:ND2	3:D:889:VAL:N	2.55	0.54
3:D:939:LEU:CD2	3:D:1016:ARG:HH11	2.20	0.54
3:A:483:GLN:NE2	3:A:489:TRP:HA	2.23	0.54
3:D:66:ILE:HD13	3:D:75:THR:HG22	1.90	0.54
3:D:344:ARG:NH1	3:D:408:LEU:HD21	2.23	0.54
1:B:61:HIS:CE1	1:B:101:GLN:HE22	2.25	0.54
3:A:73:MET:HG3	3:A:126:TYR:HB2	1.88	0.54
3:D:284:GLU:HG3	3:D:343:LEU:HD21	1.89	0.54
3:D:894:LEU:HD13	3:D:941:MET:HB2	1.90	0.54
3:A:251:ILE:HG21	3:A:289:LEU:HB3	1.89	0.54
3:D:218:ASN:HB3	3:D:221:LEU:HB3	1.89	0.54
1:B:171:ILE:O	1:B:189:MET:HG2	2.08	0.54
3:A:429:GLU:CG	3:A:445:MET:HG3	2.38	0.54
3:A:887:ARG:HD3	3:A:937:ALA:CB	2.37	0.54
3:A:888:ASN:HD22	3:A:888:ASN:N	2.04	0.54
3:D:73:MET:HG3	3:D:126:TYR:HB2	1.89	0.54
3:A:187:THR:HG23	3:A:190:LYS:H	1.73	0.54
3:A:274:VAL:HG12	3:A:275:SER:N	2.23	0.54
2:C:89:MET:HE2	2:C:120:CYS:HB2	1.90	0.54
2:C:123:LYS:HE2	5:C:217:GTP:C4	2.43	0.54
3:A:187:THR:H	3:A:190:LYS:HZ2	1.55	0.54
3:A:864:LEU:HD11	3:A:907:GLU:OE1	2.08	0.54
1:E:70:TRP:CD2	1:E:96:LYS:O	2.61	0.54
3:A:437:GLN:HB3	8:A:1267:HOH:O	2.07	0.53
3:A:672:ALA:CA	3:A:678:ILE:HD11	2.38	0.53
3:D:22:LYS:HE2	3:D:58:ASP:HB2	1.88	0.53
3:D:274:VAL:HG12	3:D:275:SER:N	2.24	0.53
3:D:390:ALA:HB3	8:D:1367:HOH:O	2.09	0.53
3:D:511:GLU:HB2	8:D:1128:HOH:O	2.07	0.53
2:F:176:PHE:HD2	2:F:176:PHE:O	1.90	0.53



30	GJ	Х
0		- <b>x</b>

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:705:PRO:O	3:D:708[A]:ILE:HG22	2.08	0.53
3:A:87:ILE:O	3:A:91:TRP:HB2	2.08	0.53
3:D:153:ILE:HD11	3:D:171:LEU:HD21	1.89	0.53
3:D:160:SER:HB3	3:D:163:LEU:HD12	1.90	0.53
1:B:138:SER:HA	1:B:159:GLY:O	2.09	0.53
3:A:30:ASN:HA	3:A:33:ASN:HD22	1.73	0.53
3:A:393:LEU:HB3	3:A:399:HIS:ND1	2.23	0.53
3:D:256:ASN:HB3	3:D:293:GLN:NE2	2.22	0.53
1:B:171:ILE:HG22	1:B:189:MET:HG3	1.90	0.53
1:B:352:ASP:HB3	3:A:711:GLY:O	2.08	0.53
2:F:28:LYS:HG2	8:F:745:HOH:O	2.08	0.53
3:D:284:GLU:CD	3:D:343:LEU:HD11	2.29	0.53
3:D:716:ASP:O	3:D:720:VAL:HG13	2.09	0.53
3:A:187:THR:H	3:A:190:LYS:NZ	2.07	0.53
3:A:32:VAL:HG22	3:A:71:GLN:CB	2.38	0.53
3:A:299:PRO:HB2	3:A:302:THR:HG23	1.89	0.53
3:A:739:VAL:HG12	3:A:745[A]:ILE:HG13	1.89	0.53
3:D:299:PRO:HB2	3:D:302:THR:HG23	1.89	0.53
3:A:153:ILE:HD11	3:A:171:LEU:HD21	1.90	0.53
3:D:87:ILE:O	3:D:91:TRP:HB2	2.08	0.53
3:D:1033:LEU:HB2	3:D:1035:LEU:HG	1.91	0.53
3:A:84:GLU:O	3:A:88:LYS:HG3	2.08	0.53
3:A:142:TRP:HB3	3:A:143:PRO:HD3	1.90	0.53
3:D:912:GLN:O	3:D:916[B]:GLN:HG3	2.09	0.53
3:D:887:ARG:HD3	3:D:937:ALA:CB	2.39	0.52
3:D:393:LEU:HD21	3:D:397:SER:HB3	1.90	0.52
1:B:187:ASP:OD1	1:B:204:ARG:HD2	2.10	0.52
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.44	0.52
3:A:437:GLN:HG2	3:A:746:ARG:CG	2.39	0.52
3:A:962:LEU:HD13	3:A:973:PHE:CE2	2.43	0.52
3:A:990:GLN:HG2	3:A:993:GLN:HE21	1.74	0.52
1:E:104:LEU:O	1:E:270:SER:HA	2.09	0.52
3:D:1029:ASP:OD1	3:D:1029:ASP:N	2.42	0.52
3:A:142:TRP:O	3:A:146:TRP:HB3	2.09	0.52
2:F:89:MET:HE2	2:F:120:CYS:HB2	1.91	0.52
3:A:285:THR:O	3:A:289:LEU:HD13	2.08	0.52
3:A:724:LEU:HD12	3:A:751:VAL:HG11	1.90	0.52
3:A:960:THR:HG22	3:A:963:ASN:H	1.74	0.52
3:D:142:TRP:HB3	3:D:143:PRO:HD3	1.90	0.52
3:D:212:VAL:O	3:D:216:SER:HB3	2.09	0.52
3:D:672:ALA:CA	3:D:678:ILE:HD11	2.39	0.52



30	GJ	Х
0		- <b>x</b>

A + 1	A + 9	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:A:284:GLU:CD	3:A:343:LEU:HD11	2.30	0.52
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.40	0.52
2:F:29:ARG:CB	2:F:157:PHE:HZ	2.14	0.52
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.44	0.52
3:D:735:ASN:HB2	3:D:739:VAL:CG2	2.40	0.52
1:E:352:ASP:HB2	3:D:711:GLY:O	2.09	0.52
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.45	0.52
3:D:957:LYS:HZ3	3:D:961:PRO:HB3	1.74	0.52
1:E:358:MET:O	1:E:359:GLU:HB2	2.10	0.52
3:D:141:GLU:HG2	3:D:145[A]:HIS:CD2	2.43	0.52
1:E:172:LEU:HD22	1:E:188[B]:VAL:HG12	1.92	0.52
3:D:960:THR:HG22	3:D:963:ASN:H	1.75	0.52
3:D:990:GLN:HG2	3:D:993:GLN:HE21	1.74	0.52
3:D:105:TYR:O	3:D:109:LEU:HG	2.10	0.52
3:D:963:ASN:N	3:D:964:PRO:CD	2.73	0.51
3:A:566:VAL:HG11	3:A:610:PHE:HE2	1.74	0.51
3:D:127:ILE:HD12	3:D:127:ILE:N	2.25	0.51
3:D:476:MET:CE	3:D:516:PHE:CZ	2.93	0.51
3:D:821:GLN:OE1	3:D:821:GLN:HA	2.10	0.51
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.11	0.51
3:A:333:HIS:HB3	3:A:336:LEU:HD23	1.92	0.51
3:D:437:GLN:HG2	3:D:746:ARG:CG	2.39	0.51
1:B:128:LYS:O	1:B:175:ILE:HA	2.11	0.51
3:A:912:GLN:NE2	3:A:958:ILE:HG23	2.25	0.51
2:F:59:ILE:HD13	2:F:60:LYS:N	2.25	0.51
1:B:59:VAL:HA	1:B:195:PRO:HG2	1.91	0.51
3:D:131:ASN:HD21	3:D:166:ASN:ND2	1.90	0.51
3:A:212:VAL:O	3:A:216:SER:HB3	2.10	0.51
1:E:188[A]:VAL:HG13	1:E:188[A]:VAL:O	2.10	0.51
3:D:788:TYR:CD2	3:D:826:VAL:HG12	2.45	0.51
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.91	0.51
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.46	0.51
3:A:509[B]:HIS:HD2	3:A:511:GLU:HB3	1.71	0.51
1:E:44:ARG:NH2	1:E:272:PRO:HG3	2.26	0.51
3:D:305:ARG:HG3	8:D:1384:HOH:O	2.11	0.51
3:D:434:GLU:HA	3:D:439:GLU:O	2.10	0.51
3:D:436:ASP:O	3:D:437:GLN:HG3	2.11	0.51
3:D:518:VAL:O	3:D:522:LYS:HB2	2.10	0.51
3:D:912:GLN:NE2	3:D:958:ILE:HG23	2.25	0.51
3:A:110:ILE:HD13	3:A:130:LEU:HD13	1.93	0.51
3:A:664:VAL:CG1	3:A:691:ILE:HD11	2.40	0.51



30	GJ	Х
0		- <b>x</b>

	• <u>r</u>	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:353:HIS:N	1:B:353:HIS:CD2	2.79	0.51
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.46	0.51
3:A:755:THR:O	3:A:759:ILE:HG13	2.11	0.51
3:D:104:LYS:HA	3:D:107:VAL:HG22	1.92	0.51
3:D:429:GLU:HA	3:D:429:GLU:OE1	2.10	0.51
3:A:851:LEU:O	3:A:855:VAL:HG23	2.11	0.51
1:E:356:CYS:HB3	3:D:673:THR:OG1	2.11	0.51
3:D:19:PHE:O	3:D:19:PHE:CD1	2.64	0.51
2:C:98:TYR:O	2:C:101:VAL:HG23	2.11	0.50
3:D:58:ASP:CG	3:D:62:ARG:HE	2.14	0.50
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
1:B:57:ASP:OD1	1:B:59:VAL:HB	2.10	0.50
3:A:105:TYR:O	3:A:109:LEU:HG	2.11	0.50
3:A:129:LYS:O	3:A:133:ILE:HG13	2.11	0.50
3:A:887:ARG:NH2	3:A:891:ASP:HB3	2.25	0.50
3:A:1048:GLU:O	3:A:1052:LEU:N	2.45	0.50
1:E:187:ASP:HB3	1:E:189:MET:HE1	1.93	0.50
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.92	0.50
3:D:881:ALA:O	3:D:884:HIS:HB2	2.11	0.50
3:D:887:ARG:NH2	3:D:891:ASP:HB3	2.25	0.50
1:B:106[B]:GLU:O	1:B:275:GLY:HA2	2.12	0.50
2:C:32:THR:OG1	2:C:34:GLU:HG2	2.11	0.50
3:A:276:VAL:HB	3:A:333:HIS:ND1	2.25	0.50
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.93	0.50
2:F:176:PHE:O	2:F:176:PHE:CD2	2.64	0.50
2:C:129:ARG:NH1	3:A:447:ASP:O	2.45	0.50
1:E:59:VAL:HA	1:E:195:PRO:HG2	1.92	0.50
3:D:333:HIS:HB3	3:D:336:LEU:HD23	1.93	0.50
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
3:D:996:LEU:O	3:D:999:THR:HG22	2.11	0.50
1:E:225:ASN:N	1:E:226:PRO:HD3	2.27	0.50
3:D:66:ILE:CD1	3:D:75:THR:HG22	2.42	0.50
3:D:566:VAL:HG11	3:D:610:PHE:HE2	1.75	0.50
3:D:1050:HIS:HA	3:D:1053:GLN:HG2	1.92	0.50
3:A:123:GLU:OE1	3:A:123:GLU:HA	2.11	0.50
2:F:38:LYS:HG2	3:D:842:PRO:HG3	1.94	0.50
3:D:755:THR:O	3:D:759:ILE:HG13	2.12	0.50
1:B:202:ASP:HB3	1:B:262:LYS:HG2	1.94	0.50
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.76	0.50
3:D:1008:ILE:CG2	3:D:1009:PRO:HD3	2.30	0.50
2:C:29:ARG:CB	2:C:157:PHE:HZ	2.15	0.50



30	GJ	Х
0		- <b>x</b>

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:483:GLN:NE2	3:D:489:TRP:HA	2.26	0.50
2:C:52:PHE:HE1	2:C:61:PHE:HD2	1.60	0.50
3:D:729:SER:OG	3:D:792:VAL:HG22	2.12	0.50
2:C:59:ILE:HD13	2:C:60:LYS:N	2.26	0.49
3:A:181:PHE:O	3:A:185:GLN:HG2	2.12	0.49
3:A:559:TRP:CD2	3:A:603:GLN:HG3	2.46	0.49
3:A:968:VAL:HG12	3:A:973:PHE:HB2	1.93	0.49
1:B:215:GLU:O	1:B:216:GLU:C	2.50	0.49
3:A:393:LEU:HD22	3:A:398:GLN:CA	2.35	0.49
3:A:957:LYS:HZ3	3:A:961:PRO:HB3	1.75	0.49
3:D:326:LEU:O	3:D:330:LEU:HG	2.12	0.49
3:A:894:LEU:HD13	3:A:941:MET:HB2	1.95	0.49
1:E:25:HIS:HE1	1:E:27:ARG:HD3	1.78	0.49
1:E:57:ASP:OD1	1:E:59:VAL:HB	2.11	0.49
2:F:29:ARG:HG2	2:F:34:GLU:O	2.12	0.49
3:D:175[B]:SER:OG	3:D:232:PHE:HE1	1.95	0.49
3:D:476:MET:HE2	3:D:516:PHE:HZ	1.77	0.49
3:D:788:TYR:O	3:D:796:ARG:HG2	2.12	0.49
1:B:8:LEU:HD22	3:A:564:THR:HG22	1.93	0.49
1:E:358:MET:O	1:E:359:GLU:CB	2.60	0.49
3:D:129:LYS:O	3:D:133:ILE:HG13	2.12	0.49
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.48	0.49
3:D:435:ASN:CG	3:D:439:GLU:HB2	2.32	0.49
1:B:70:TRP:CD1	1:B:97:HIS:CE1	3.00	0.49
1:B:222:THR:HG22	1:B:225:ASN:N	2.26	0.49
3:A:875:LEU:O	3:A:879:ILE:HG12	2.13	0.49
3:D:30:ASN:HB3	3:D:44:ARG:HD2	1.94	0.49
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.47	0.49
3:D:344:ARG:O	3:D:348:MET:HG2	2.12	0.49
3:D:882:PHE:CD1	3:D:882:PHE:C	2.86	0.49
3:A:26:ASN:HB3	8:A:1204:HOH:O	2.12	0.49
3:A:996:LEU:O	3:A:999:THR:HG22	2.12	0.49
3:D:56:HIS:O	3:D:56:HIS:CD2	2.66	0.49
3:D:797:GLU:OE2	3:D:798:PRO:HD2	2.13	0.49
3:D:875:LEU:O	3:D:879:ILE:HG12	2.13	0.49
3:A:76:LYS:HB3	3:A:126:TYR:CE1	2.47	0.49
3:A:187:THR:CG2	3:A:190:LYS:HB2	2.43	0.49
3:A:967:PRO:HG2	3:A:968:VAL:HG23	1.95	0.49
2:F:86:ALA:HB3	2:F:108:LEU:HD21	1.94	0.49
3:D:142:TRP:O	3:D:146:TRP:HB3	2.12	0.49
2:C:86:ALA:HB3	2:C:108:LEU:HD21	1.93	0.49



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:990:GLN:H	3:A:993:GLN:NE2	2.04	0.49
2:C:47:VAL:HG13	2:C:47:VAL:O	2.12	0.49
3:A:882:PHE:C	3:A:882:PHE:CD1	2.86	0.49
1:E:114:ASP:HB3	8:E:876:HOH:O	2.13	0.49
3:D:28:LEU:HD12	3:D:75:THR:OG1	2.13	0.49
3:D:54:LYS:O	3:D:55:GLU:HG2	2.13	0.49
3:D:276:VAL:HB	3:D:333:HIS:ND1	2.27	0.49
1:E:219:GLY:O	1:E:228:LYS:HD2	2.13	0.49
3:D:1033:LEU:CD1	3:D:1035:LEU:HD21	2.43	0.49
3:A:429:GLU:OE1	3:A:429:GLU:HA	2.12	0.48
3:A:435:ASN:C	3:A:437:GLN:H	2.16	0.48
1:E:350:SER:CB	1:E:351:PRO:HD2	2.17	0.48
3:D:988:HIS:CD2	3:D:988:HIS:H	2.31	0.48
3:A:545:MET:SD	3:A:569:LEU:HD11	2.52	0.48
3:D:208:LEU:C	3:D:208:LEU:HD23	2.33	0.48
3:D:406:ARG:HD3	8:D:1182:HOH:O	2.13	0.48
3:A:23:LEU:H	3:A:23:LEU:CD1	2.26	0.48
3:A:56:HIS:O	3:A:56:HIS:CD2	2.66	0.48
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.48	0.48
3:D:357:VAL:HG13	3:D:369:CYS:SG	2.53	0.48
3:D:429:GLU:CG	3:D:445:MET:HG3	2.42	0.48
3:D:841:TYR:O	3:D:845:ARG:HG3	2.13	0.48
2:C:29:ARG:HG2	2:C:34:GLU:O	2.14	0.48
3:D:517:LEU:HD11	3:D:551:TYR:CD1	2.47	0.48
1:B:44:ARG:NH2	1:B:272:PRO:HG3	2.29	0.48
3:A:27:LEU:O	3:A:31:VAL:HG23	2.14	0.48
3:A:344:ARG:O	3:A:348:MET:HG2	2.13	0.48
3:A:962:LEU:CD2	3:A:968:VAL:HG11	2.40	0.48
1:E:283:SER:O	1:E:288:VAL:HG13	2.14	0.48
2:F:52:PHE:HE1	2:F:61:PHE:HD2	1.61	0.48
2:F:81:ILE:O	2:F:82:GLN:HB2	2.13	0.48
2:F:156:ASN:ND2	2:F:159:LYS:HZ1	2.11	0.48
3:D:486:GLY:O	3:D:487:THR:C	2.51	0.48
2:C:125:ASP:O	2:C:127:LYS:HE3	2.13	0.48
3:A:518:VAL:O	3:A:522:LYS:HB2	2.12	0.48
3:A:881:ALA:O	3:A:884:HIS:HB2	2.13	0.48
1:E:289:ALA:O	1:E:290:VAL:HB	2.13	0.48
3:D:145[A]:HIS:C	3:D:147:PRO:HD3	2.33	0.48
3:D:268:LEU:HD22	3:D:286:LEU:HD11	1.95	0.48
1:B:104:LEU:O	1:B:270:SER:HA	2.13	0.48
2:C:178:ALA:O	2:C:179:MET:HB2	2.14	0.48



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:76:LYS:HB3	3:A:126:TYR:HE1	1.78	0.48
3:A:953:VAL:CG2	3:A:974:ILE:HD12	2.43	0.48
3:D:354:MET:HB3	3:D:373:TRP:CZ2	2.49	0.48
3:D:838:PHE:HA	3:D:845:ARG:NH2	2.29	0.48
1:B:60:ASN:O	1:B:64:ARG:HG3	2.14	0.48
3:A:23:LEU:HD13	3:A:26:ASN:HB2	1.96	0.48
3:A:62:ARG:HH11	3:A:79:GLY:CA	2.17	0.48
3:A:993:GLN:HG2	3:A:1033:LEU:HD22	1.96	0.48
3:D:27:LEU:O	3:D:31:VAL:HG23	2.14	0.48
3:D:52:HIS:CE1	3:D:82:ILE:HD12	2.49	0.48
3:D:120:VAL:HG23	3:D:121:GLU:N	2.28	0.48
3:D:185:GLN:HG3	3:D:186:ILE:HG13	1.95	0.48
3:A:104:LYS:HA	3:A:107:VAL:HG22	1.95	0.48
3:A:136:GLN:OE1	3:A:136:GLN:HA	2.14	0.48
3:D:175[B]:SER:OG	3:D:232:PHE:CE1	2.66	0.48
3:D:181:PHE:O	3:D:185:GLN:HG2	2.13	0.48
2:C:31:LEU:CD1	2:C:32:THR:HG23	2.44	0.47
3:A:578:ASP:HA	8:A:1148:HOH:O	2.13	0.47
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.14	0.47
1:B:245:VAL:HA	1:B:248:MET:SD	2.54	0.47
2:C:86:ALA:CB	2:C:108:LEU:HD21	2.44	0.47
1:E:204:ARG:HA	8:E:492:HOH:O	2.13	0.47
1:E:358:MET:HB3	1:E:359:GLU:H	1.39	0.47
3:D:739:VAL:HG12	3:D:745:ILE:HG13	1.95	0.47
3:A:486:GLY:O	3:A:487:THR:C	2.52	0.47
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.97	0.47
2:C:15:LEU:HD22	2:C:23:LYS:HD2	1.96	0.47
1:E:43:ARG:HE	1:E:43:ARG:HB3	1.41	0.47
3:D:511:GLU:HG2	3:D:515:ARG:NH1	2.29	0.47
3:D:607:VAL:HG23	3:D:608:MET:HG2	1.96	0.47
2:C:52:PHE:CE1	2:C:61:PHE:HD2	2.32	0.47
3:A:28:LEU:HD12	3:A:75:THR:OG1	2.14	0.47
3:A:716:ASP:O	3:A:720:VAL:HG13	2.15	0.47
3:A:960:THR:HA	3:A:961:PRO:HD3	1.74	0.47
1:B:171:ILE:HG22	1:B:189:MET:CG	2.45	0.47
3:A:122:LYS:O	3:A:123:GLU:O	2.33	0.47
3:A:424:MET:HA	3:A:457:MET:CE	2.44	0.47
3:A:688:LEU:O	3:A:692:LEU:HG	2.14	0.47
3:A:953:VAL:HG21	3:A:974:ILE:HD12	1.97	0.47
3:A:962:LEU:O	3:A:963:ASN:CB	2.61	0.47
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.96	0.47



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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:257:VAL:HG21	3:D:260:PHE:CD2	2.48	0.47
3:D:344:ARG:CZ	3:D:408:LEU:HD11	2.44	0.47
3:D:399:HIS:C	3:D:401:ASP:N	2.68	0.47
3:D:664:VAL:CG1	3:D:691:ILE:HD11	2.45	0.47
1:B:42:GLU:HB3	8:B:948:HOH:O	2.14	0.47
1:B:128:LYS:HG3	1:B:176:TYR:HB3	1.96	0.47
3:A:257:VAL:HG21	3:A:260:PHE:CD2	2.49	0.47
3:A:326:LEU:O	3:A:330:LEU:HG	2.15	0.47
1:E:126:VAL:HG13	1:E:253:GLU:HB2	1.95	0.47
2:F:88:ILE:HG21	2:F:101:VAL:HG13	1.96	0.47
3:D:996:LEU:HD22	3:D:1035:LEU:HD23	1.97	0.47
3:A:185:GLN:HG3	3:A:186:ILE:HG13	1.96	0.47
3:D:135:VAL:HG12	3:D:139:LYS:HE2	1.96	0.47
3:D:688:LEU:O	3:D:692:LEU:HG	2.14	0.47
1:B:219:GLY:O	1:B:228:LYS:HD2	2.15	0.47
3:A:988:HIS:H	3:A:988:HIS:CD2	2.32	0.47
3:D:136:GLN:HA	3:D:136:GLN:OE1	2.15	0.47
3:D:436:ASP:C	3:D:437:GLN:HG3	2.34	0.47
3:D:453:LEU:O	3:D:457:MET:HG3	2.15	0.47
2:C:88:ILE:HG21	2:C:101:VAL:HG13	1.96	0.46
3:A:73:MET:CG	3:A:126:TYR:HB2	2.45	0.46
3:A:453:LEU:O	3:A:457:MET:HG3	2.15	0.46
3:A:837:ASP:O	3:A:845:ARG:NH2	2.46	0.46
3:D:953:VAL:CG2	3:D:974:ILE:HD12	2.45	0.46
1:B:29:SER:O	1:B:30:GLN:C	2.52	0.46
3:A:788:TYR:O	3:A:796:ARG:HG2	2.15	0.46
1:E:25:HIS:CE1	1:E:27:ARG:HD3	2.50	0.46
3:D:35:LEU:HD12	3:D:71:GLN:OE1	2.14	0.46
3:D:327:CYS:HB2	3:D:354:MET:CE	2.45	0.46
2:C:91:ASP:OD1	2:C:123:LYS:HD2	2.15	0.46
3:A:139:LYS:HD3	3:A:186:ILE:HD11	1.97	0.46
3:A:146:TRP:CD2	3:A:149:PHE:HB2	2.50	0.46
3:A:962:LEU:HB2	3:A:973:PHE:CE2	2.50	0.46
1:E:176:TYR:HB2	1:E:183:TYR:CD1	2.50	0.46
3:D:73:MET:CG	3:D:126:TYR:HB2	2.45	0.46
3:D:202:PHE:CZ	3:D:236:ILE:HG21	2.51	0.46
3:D:760:SER:HB3	3:D:803:THR:HG23	1.98	0.46
1:B:106[A]:GLU:HG3	1:B:271:THR:O	2.15	0.46
2:C:81:ILE:O	2:C:82:GLN:HB2	2.15	0.46
3:A:96:ARG:NH2	3:A:145:HIS:CG	2.83	0.46
3:A:476:MET:CE	3:A:516:PHE:CZ	2.94	0.46



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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:A:517:LEU:HD11	3:A:551:TYR:CD1	2.50	0.46
3:A:721:TYR:C	3:A:721:TYR:CD2	2.88	0.46
3:A:788:TYR:CD2	3:A:826:VAL:HG12	2.50	0.46
1:E:265:HIS:CE1	8:E:497:HOH:O	2.68	0.46
3:D:435:ASN:HD21	3:D:439:GLU:HB2	1.77	0.46
3:A:239:GLY:O	3:A:243:GLU:HB2	2.15	0.46
3:A:525:LEU:CD1	3:A:544:ILE:HD13	2.46	0.46
1:E:52[A]:LYS:HD3	1:E:265:HIS:CG	2.50	0.46
2:F:36:GLU:OE2	2:F:38:LYS:HE3	2.16	0.46
3:D:24:ASP:OD2	3:D:62:ARG:HA	2.16	0.46
3:D:716:ASP:O	3:D:720:VAL:CG1	2.64	0.46
3:D:721:TYR:CD2	3:D:721:TYR:C	2.89	0.46
3:D:739:VAL:O	3:D:742:GLN:HG2	2.16	0.46
1:B:285:VAL:O	1:B:286:LEU:HD12	2.16	0.46
3:A:124:LYS:H	3:A:124:LYS:HD2	1.81	0.46
3:A:668:ILE:HG12	8:A:1279:HOH:O	2.15	0.46
3:A:797:GLU:OE2	3:A:798:PRO:HD2	2.16	0.46
2:F:122:ASN:O	2:F:123:LYS:HB2	2.15	0.46
2:C:178:ALA:O	2:C:179:MET:CB	2.63	0.46
3:A:509[B]:HIS:HD2	3:A:511:GLU:N	2.09	0.46
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.98	0.46
1:E:349:HIS:NE2	3:D:708[A]:ILE:HD12	2.31	0.46
2:F:53:HIS:O	2:F:176:PHE:HB2	2.15	0.46
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.97	0.46
3:A:106:VAL:O	3:A:110:ILE:HG12	2.15	0.46
3:A:268:LEU:HD22	3:A:286:LEU:HD11	1.97	0.46
3:A:307:ALA:O	3:A:315:GLU:OE2	2.34	0.46
3:A:393:LEU:CD2	3:A:398:GLN:HA	2.39	0.46
3:A:678:ILE:C	3:A:680:LYS:N	2.69	0.46
1:E:212:LEU:N	1:E:213:PRO:CD	2.79	0.46
3:D:119:CYS:SG	3:D:127:ILE:HG12	2.56	0.46
3:D:217:GLN:HE21	3:D:217:GLN:HB2	1.54	0.46
3:D:815:ILE:HA	3:D:818:GLU:OE1	2.16	0.46
3:D:124:LYS:H	3:D:124:LYS:HD2	1.81	0.46
3:D:485:ASN:C	3:D:487:THR:N	2.68	0.46
3:D:982:LEU:HD13	3:D:1018:PHE:CZ	2.51	0.46
1:B:52:LYS:HD3	1:B:265:HIS:ND1	2.30	0.45
1:B:208:MET:HG2	1:B:212:LEU:CD1	2.46	0.45
1:B:209:HIS:O	1:B:213:PRO:HG2	2.16	0.45
1:E:359:GLU:HB3	3:D:722:LYS:HD3	1.98	0.45
2:F:52:PHE:CE1	2:F:61:PHE:HD2	2.33	0.45



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:678:ILE:C	3:D:680:LYS:N	2.69	0.45
3:D:829:CYS:O	3:D:833:MET:HG3	2.16	0.45
3:A:440:VAL:O	3:A:440:VAL:HG23	2.16	0.45
3:A:815:ILE:HA	3:A:818:GLU:OE1	2.16	0.45
1:E:189:MET:O	1:E:196:PHE:N	2.43	0.45
1:E:360:ASN:O	1:E:360:ASN:CG	2.54	0.45
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.97	0.45
3:D:600:VAL:HG13	3:D:644:GLN:NE2	2.30	0.45
3:D:953:VAL:HG21	3:D:974:ILE:HD12	1.98	0.45
3:A:611:ILE:HG13	3:A:615[B]:LEU:HD22	1.99	0.45
3:D:402:ILE:HG21	3:D:407:GLN:NE2	2.31	0.45
3:D:424:MET:HA	3:D:457:MET:CE	2.45	0.45
3:D:497:LEU:HD12	3:D:497:LEU:O	2.16	0.45
3:D:544:ILE:HG22	3:D:545:MET:CE	2.46	0.45
3:D:654:ILE:HB	3:D:708[B]:ILE:HD11	1.99	0.45
3:A:186:ILE:HG22	3:A:187:THR:O	2.17	0.45
3:A:829:CYS:O	3:A:833:MET:HG3	2.17	0.45
2:F:77:ASP:N	2:F:77:ASP:OD1	2.50	0.45
2:F:81:ILE:HD11	3:D:77:TYR:CD2	2.51	0.45
3:D:290:THR:HG21	3:D:325:PHE:CZ	2.51	0.45
1:B:225:ASN:N	1:B:226:PRO:HD3	2.32	0.45
3:A:223:HIS:CE1	3:A:263:VAL:HG21	2.51	0.45
3:A:739:VAL:O	3:A:742:GLN:HG2	2.17	0.45
2:F:98:TYR:O	2:F:101:VAL:HG23	2.17	0.45
3:D:593:GLN:HB3	8:D:1328:HOH:O	2.16	0.45
3:D:665:TRP:CZ3	3:D:692:LEU:HD21	2.50	0.45
1:B:160:ASN:O	1:B:161:ARG:HB2	2.17	0.45
3:A:70:SER:O	3:A:71:GLN:HB2	2.16	0.45
1:E:129:ARG:HG2	1:E:144:LYS:HE3	1.98	0.45
1:E:173:ASP:HB2	1:E:189:MET:CE	2.46	0.45
2:C:123:LYS:HG2	5:C:217:GTP:C6	2.51	0.45
3:A:485:ASN:C	3:A:487:THR:N	2.69	0.45
1:E:209:HIS:HE1	1:E:232:LEU:O	1.99	0.45
3:D:146:TRP:CD2	3:D:149:PHE:HB2	2.52	0.45
1:B:209:HIS:NE2	1:B:232:LEU:O	2.50	0.45
1:B:212:LEU:N	1:B:213:PRO:CD	2.79	0.45
3:A:19:PHE:CG	3:A:19:PHE:O	2.70	0.45
3:A:940:THR:O	3:A:944:SER:HB2	2.17	0.45
3:D:480:LEU:O	3:D:483:GLN:HB2	2.16	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.47	0.45
1:B:264:THR:OG1	1:B:273:LEU:HB3	2.17	0.45



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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:95:ARG:NH1	2:C:130:LYS:HE2	2.32	0.45
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.99	0.45
1:E:41:SER:HB2	1:E:110:ASP:HB3	1.97	0.45
3:D:989:LEU:HD11	3:D:1022:ILE:HG22	1.99	0.45
1:B:7:ALA:HA	8:B:410:HOH:O	2.16	0.45
2:C:156:ASN:ND2	2:C:159:LYS:HZ1	2.15	0.45
3:A:95:PRO:HG2	3:A:98:GLN:HB2	1.99	0.45
3:A:110:ILE:HD11	3:A:130:LEU:HB3	1.96	0.45
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.99	0.45
3:A:989:LEU:HD11	3:A:1022:ILE:HG22	1.99	0.45
2:F:86:ALA:CB	2:F:108:LEU:HD21	2.47	0.45
3:D:127:ILE:N	3:D:127:ILE:CD1	2.80	0.45
3:D:772:VAL:HG12	3:D:811:LEU:HD11	1.98	0.45
3:D:962:LEU:O	3:D:963:ASN:HB2	2.17	0.45
1:B:57:ASP:HB3	8:B:903:HOH:O	2.16	0.44
1:B:285:VAL:O	1:B:286:LEU:HB2	2.17	0.44
3:A:274:VAL:HG12	3:A:275:SER:H	1.82	0.44
1:E:8:LEU:HD22	3:D:564:THR:HG22	1.99	0.44
1:B:208:MET:HG2	1:B:212:LEU:HD11	1.98	0.44
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.98	0.44
3:A:55:GLU:HG2	3:A:56:HIS:N	2.28	0.44
3:A:534:LYS:HB3	3:A:577:HIS:CD2	2.51	0.44
1:E:187:ASP:OD1	1:E:204:ARG:HD2	2.17	0.44
3:A:287:PHE:HB2	3:A:329:PHE:CZ	2.51	0.44
1:E:180:ASN:O	1:E:181:GLN:C	2.53	0.44
2:F:38:LYS:HE3	2:F:38:LYS:HB2	1.77	0.44
3:D:216:SER:HB2	3:D:222:VAL:HG22	1.99	0.44
3:D:693:LYS:O	3:D:697:ARG:HG2	2.17	0.44
3:A:30:ASN:CA	3:A:44:ARG:HD2	2.48	0.44
3:A:594:LYS:HE2	3:A:594:LYS:HA	2.00	0.44
1:E:97[A]:HIS:CD2	1:E:98:TYR:N	2.85	0.44
3:D:53:LEU:CD1	3:D:54:LYS:H	2.19	0.44
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.82	0.44
3:D:966:ASN:N	3:D:967:PRO:HD2	2.33	0.44
3:D:218:ASN:O	3:D:222:VAL:HG23	2.18	0.44
3:D:716:ASP:HA	8:D:1253:HOH:O	2.16	0.44
3:A:600:VAL:HG13	3:A:644:GLN:NE2	2.32	0.44
3:A:693:LYS:O	3:A:697:ARG:HG2	2.18	0.44
3:A:1046:GLN:OE1	3:A:1049:LYS:HD3	2.17	0.44
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.44
3:D:257:VAL:HG22	3:D:260:PHE:HB2	2.00	0.44



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:402:ILE:O	3:D:402:ILE:HG23	2.17	0.44
3:D:458:ARG:HG3	3:D:503:SER:HB2	2.00	0.44
1:B:58:TYR:HB3	1:B:197:TYR:HD1	1.83	0.44
3:A:437:GLN:C	3:A:439:GLU:H	2.21	0.44
3:A:607:VAL:HG23	3:A:608:MET:HG2	1.99	0.44
1:E:12:PHE:HE2	3:D:545:MET:HE3	1.83	0.44
3:D:685:VAL:HA	3:D:688:LEU:HD12	2.00	0.44
3:D:849:PHE:CZ	3:D:881:ALA:HB2	2.52	0.44
1:B:176:TYR:HB2	1:B:183:TYR:CD1	2.52	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG22	2.00	0.44
3:A:277:SER:HB3	3:A:278:GLN:OE1	2.18	0.44
3:A:388:THR:HG22	3:A:389:SER:H	1.81	0.44
3:A:414:SER:OG	3:A:471:ASP:OD2	2.32	0.44
1:E:-1:GLY:O	1:E:3[A]:GLU:HG2	2.17	0.44
1:E:240:GLU:CD	1:E:240:GLU:H	2.20	0.44
2:F:123:LYS:HG2	5:F:217:GTP:C6	2.53	0.44
3:D:17:LEU:HA	3:D:17:LEU:HD12	1.76	0.44
3:D:887:ARG:HD2	3:D:887:ARG:HA	1.58	0.44
3:D:1038:ARG:O	3:D:1042:LEU:HG	2.18	0.44
3:A:186:ILE:HG23	3:A:190:LYS:HD2	1.99	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG21	2.00	0.44
3:A:286:LEU:HD12	3:A:286:LEU:O	2.18	0.44
1:E:208:MET:HG2	1:E:212:LEU:CD1	2.48	0.44
3:D:223:HIS:CE1	3:D:263:VAL:HG21	2.52	0.44
3:D:731:ALA:HB1	3:D:739:VAL:HG11	1.99	0.44
2:C:91:ASP:CG	2:C:123:LYS:HD2	2.38	0.43
1:E:102:LEU:CD1	1:E:129:ARG:HG3	2.48	0.43
2:F:40:VAL:HG13	3:D:839:GLU:OE1	2.18	0.43
2:F:91:ASP:OD1	2:F:123:LYS:HD2	2.18	0.43
3:D:22:LYS:HB2	3:D:61:THR:HG21	1.98	0.43
3:D:66:ILE:HD13	3:D:75:THR:CG2	2.48	0.43
1:B:253:GLU:H	1:B:253:GLU:HG3	1.66	0.43
3:A:94:LEU:HD22	3:A:98:GLN:HG2	1.99	0.43
3:A:223:HIS:CE1	3:A:263:VAL:CG2	3.01	0.43
3:D:274:VAL:HG12	3:D:275:SER:H	1.83	0.43
3:D:393:LEU:HD12	3:D:395:SER:N	2.23	0.43
3:D:397:SER:O	3:D:398:GLN:HB2	2.18	0.43
3:A:294:LEU:HD21	3:A:322:LEU:HD11	1.99	0.43
3:A:738:MET:C	3:A:740:THR:H	2.21	0.43
3:A:993:GLN:HG2	3:A:1033:LEU:CD2	2.48	0.43
1:E:351:PRO:O	1:E:352:ASP:OD1	2.37	0.43



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	• Fugen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:186:ILE:HG22	3:D:187:THR:O	2.18	0.43
2:C:81:ILE:HD11	3:A:77:TYR:CD2	2.53	0.43
3:A:344:ARG:CZ	3:A:408:LEU:HD11	2.48	0.43
3:A:545:MET:SD	3:A:569:LEU:CD1	3.06	0.43
1:E:212:LEU:HB2	1:E:213:PRO:HD3	2.01	0.43
3:A:24:ASP:O	3:A:28:LEU:HB2	2.17	0.43
3:A:778:PRO:HB2	3:A:779:PRO:HD3	2.01	0.43
1:E:209:HIS:O	1:E:213:PRO:HG2	2.19	0.43
1:E:215:GLU:O	1:E:216:GLU:C	2.57	0.43
3:D:435:ASN:C	3:D:437:GLN:H	2.21	0.43
2:C:45:VAL:HG22	2:C:46:GLU:N	2.33	0.43
3:D:303:ASN:HD21	3:D:305:ARG:NH2	2.15	0.43
3:D:534:LYS:HE2	3:D:577:HIS:HB2	2.00	0.43
3:D:666:ASP:O	3:D:670:GLN:HG3	2.19	0.43
3:A:218:ASN:O	3:A:222:VAL:HG23	2.19	0.43
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.34	0.43
3:A:689:GLY:O	3:A:693:LYS:HG3	2.18	0.43
3:A:820:PRO:HB2	8:A:1212:HOH:O	2.18	0.43
3:A:898:PHE:CE1	3:A:902:GLN:NE2	2.87	0.43
3:A:907:GLU:OE2	3:A:907:GLU:N	2.52	0.43
1:E:173:ASP:CB	1:E:189:MET:HE1	2.49	0.43
3:D:294:LEU:HD21	3:D:322:LEU:HD11	1.99	0.43
3:D:753:ARG:NH1	8:D:1310:HOH:O	2.51	0.43
3:D:778:PRO:HB2	3:D:779:PRO:HD3	2.01	0.43
3:D:961:PRO:HD2	3:D:962:LEU:H	1.83	0.43
1:B:25:HIS:ND1	1:B:26:PRO:HD2	2.34	0.43
2:C:169:ILE:HG22	2:C:170:GLY:N	2.31	0.43
3:A:206:PHE:CE2	3:A:244:THR:HG21	2.50	0.43
3:A:388:THR:CG2	3:A:399:HIS:HE2	2.29	0.43
2:F:142:LYS:HB2	2:F:144:LEU:HG	2.01	0.43
3:D:54:LYS:O	3:D:55:GLU:CG	2.66	0.43
1:B:2:GLU:C	1:B:2:GLU:OE2	2.56	0.43
1:B:192:ARG:O	1:B:194:HIS:CD2	2.72	0.43
2:C:142:LYS:HB2	2:C:144:LEU:HG	2.01	0.43
3:A:19:PHE:C	3:A:21:GLN:H	2.20	0.43
3:D:363:THR:O	3:D:367:LYS:HG3	2.19	0.43
1:B:356:CYS:O	3:A:719:ASN:ND2	2.52	0.43
2:C:80:TYR:O	2:C:81:ILE:C	2.57	0.43
3:A:716:ASP:O	3:A:720:VAL:CG1	2.67	0.43
3:A:720:VAL:HG22	8:A:1183:HOH:O	2.18	0.43
3:A:888:ASN:HD22	3:A:889:VAL:N	2.15	0.43



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:1038:ARG:O	3:A:1042:LEU:HG	2.19	0.43
3:D:92:LYS:HD2	3:D:1030:THR:CG2	2.49	0.43
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.34	0.43
3:D:287:PHE:HB2	3:D:329:PHE:CZ	2.53	0.43
3:D:426:LYS:CD	3:D:426:LYS:N	2.72	0.43
3:D:689:GLY:O	3:D:693:LYS:HG3	2.18	0.43
3:A:978:VAL:O	3:A:981:LEU:HB3	2.19	0.42
3:D:294:LEU:HD21	3:D:322:LEU:CD1	2.49	0.42
3:D:777:VAL:O	3:D:780:LEU:HB2	2.19	0.42
1:B:128:LYS:HE3	1:B:176:TYR:CD2	2.51	0.42
1:B:194:HIS:HA	1:B:195:PRO:HD3	1.92	0.42
2:C:9:VAL:HG13	2:C:9:VAL:O	2.19	0.42
3:A:511:GLU:HG2	3:A:515:ARG:NH1	2.34	0.42
3:A:840:GLU:O	3:A:845:ARG:HD2	2.18	0.42
3:A:1036:GLU:OE1	3:A:1037:GLU:HG3	2.18	0.42
1:E:70:TRP:CZ2	1:E:97[A]:HIS:HA	2.54	0.42
2:F:13:LEU:HB2	2:F:85:CYS:SG	2.59	0.42
3:D:202:PHE:HD1	3:D:205:ILE:HD11	1.83	0.42
3:A:290:THR:O	3:A:294:LEU:HB2	2.19	0.42
3:A:704:HIS:HB3	3:A:705:PRO:HD3	2.02	0.42
3:D:87:ILE:HD13	3:D:137:ILE:HG13	2.00	0.42
3:D:888:ASN:HD22	3:D:889:VAL:N	2.16	0.42
3:D:978:VAL:O	3:D:981:LEU:HB3	2.19	0.42
1:B:353:HIS:HA	1:B:354:PRO:HD3	1.63	0.42
2:C:36:GLU:HA	8:C:673:HOH:O	2.19	0.42
3:A:202:PHE:CZ	3:A:236:ILE:HG21	2.55	0.42
3:A:257:VAL:HG22	3:A:260:PHE:HB2	2.02	0.42
3:A:409:TYR:O	3:A:410:LEU:C	2.57	0.42
3:A:497:LEU:O	3:A:497:LEU:HD12	2.19	0.42
3:A:607:VAL:HA	8:A:1224:HOH:O	2.18	0.42
3:A:961:PRO:HD2	3:A:962:LEU:H	1.85	0.42
1:E:251:PRO:HG2	1:E:252:PHE:CD1	2.54	0.42
3:D:960:THR:CG2	3:D:968:VAL:HG11	2.29	0.42
1:B:359:GLU:O	1:B:360:ASN:C	2.58	0.42
2:C:106:ARG:NH1	2:C:107:ASP:OD1	2.52	0.42
3:A:218:ASN:HD22	3:A:218:ASN:C	2.22	0.42
3:A:281:GLU:OE2	3:A:281:GLU:HA	2.20	0.42
3:A:731:ALA:HB1	3:A:739:VAL:HG11	2.00	0.42
3:A:971:GLN:NE2	8:A:1078:HOH:O	2.51	0.42
3:A:978:VAL:HG12	3:A:998:VAL:HG22	2.02	0.42
2:F:15:LEU:HD22	2:F:23:LYS:HD2	2.01	0.42



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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:330:LEU:HB3	3:D:372:TYR:CE1	2.54	0.42
3:D:393:LEU:O	3:D:395:SER:N	2.52	0.42
3:A:665:TRP:CZ3	3:A:692:LEU:HD21	2.53	0.42
3:A:1036:GLU:HG2	3:A:1037:GLU:N	2.35	0.42
1:E:58:TYR:HB3	1:E:197:TYR:HD1	1.85	0.42
3:D:55:GLU:HB3	3:D:56:HIS:H	1.69	0.42
3:D:437:GLN:O	3:D:439:GLU:N	2.53	0.42
3:D:724:LEU:CD2	3:D:751:VAL:HG11	2.49	0.42
3:A:294:LEU:HD21	3:A:322:LEU:CD1	2.50	0.42
3:A:930:VAL:HG12	3:A:931:THR:N	2.33	0.42
3:A:982:LEU:HD13	3:A:1018:PHE:CZ	2.55	0.42
1:E:95:PRO:HB2	1:E:101:GLN:HE22	1.85	0.42
3:D:916[A]:GLN:HA	3:D:916[A]:GLN:NE2	2.34	0.42
1:B:151:ARG:NH1	8:B:384:HOH:O	2.52	0.42
3:A:87:ILE:HD13	3:A:137:ILE:HG13	2.01	0.42
3:A:327:CYS:O	3:A:331:LYS:HB2	2.20	0.42
3:D:106:VAL:O	3:D:110:ILE:HG13	2.20	0.42
3:D:481:GLN:OE1	3:D:485:ASN:ND2	2.53	0.42
3:D:482:ASN:HA	3:D:486:GLY:HA3	2.01	0.42
3:D:569:LEU:HD11	3:D:591:ILE:HD12	2.02	0.42
3:A:482:ASN:HA	3:A:486:GLY:HA3	2.01	0.42
3:A:882:PHE:HA	3:A:890:ALA:HA	2.01	0.42
1:E:52[B]:LYS:HD2	1:E:265:HIS:CG	2.55	0.42
2:F:106:ARG:NH1	2:F:107:ASP:OD1	2.52	0.42
1:B:104:LEU:HB2	1:B:270:SER:HA	2.01	0.42
1:B:123:VAL:HG22	1:B:257:LEU:CD2	2.50	0.42
3:A:231:ARG:HA	3:A:231:ARG:HD3	1.90	0.42
3:A:920:CYS:O	3:A:923:LEU:HB2	2.20	0.42
1:E:128:LYS:CE	3:D:623:CYS:O	2.68	0.42
1:E:224:LEU:HA	8:E:767:HOH:O	2.19	0.42
3:D:19:PHE:O	3:D:19:PHE:CG	2.72	0.42
3:D:286:LEU:HD12	3:D:286:LEU:O	2.19	0.42
3:A:123:GLU:C	3:A:125:VAL:N	2.73	0.41
3:A:685:VAL:HA	3:A:688:LEU:HD12	2.02	0.41
1:E:208:MET:HG2	1:E:212:LEU:HD11	2.01	0.41
1:E:278:ARG:HB2	1:E:281:MET:HG3	2.01	0.41
2:F:88:ILE:HB	2:F:119:LEU:HD23	2.02	0.41
3:D:104:LYS:HA	3:D:104:LYS:HD2	1.76	0.41
3:D:216:SER:HB2	3:D:222:VAL:HG21	2.02	0.41
1:B:153:SER:O	1:B:226:PRO:HD2	2.20	0.41
3:A:23:LEU:HD12	3:A:23:LEU:N	2.35	0.41



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	F	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:23:LEU:HD13	3:A:26:ASN:CB	2.50	0.41
3:A:246:LEU:O	3:A:250:LEU:HG	2.20	0.41
3:A:1054:MET:HA	8:A:1213:HOH:O	2.19	0.41
1:E:121:VAL:CG2	1:E:257:LEU:HB3	2.50	0.41
3:D:95:PRO:HG2	3:D:98:GLN:HB2	2.02	0.41
3:D:403:PRO:HA	3:D:404:PRO:HD3	1.83	0.41
3:D:738:MET:C	3:D:740:THR:H	2.22	0.41
3:A:103:LYS:HZ2	3:A:103:LYS:HB2	1.85	0.41
3:A:114:SER:C	3:A:116:ASP:H	2.23	0.41
3:A:251:ILE:HD13	3:A:289:LEU:HB2	2.02	0.41
3:A:849:PHE:CZ	3:A:881:ALA:HB2	2.54	0.41
3:D:57:PRO:HA	3:D:60:TRP:CZ3	2.55	0.41
3:D:338:GLU:OE2	3:D:409:TYR:HE2	2.03	0.41
2:C:9:VAL:O	2:C:9:VAL:HG22	2.20	0.41
2:C:39:TYR:HA	8:C:555:HOH:O	2.20	0.41
3:A:574:HIS:HD2	3:A:624:ASP:CG	2.24	0.41
3:D:920:CYS:O	3:D:923:LEU:HB2	2.21	0.41
3:A:308:TYR:CE1	3:A:365:ILE:HD11	2.55	0.41
3:A:403:PRO:HA	3:A:404:PRO:HD3	1.84	0.41
3:A:1003:SER:HA	3:A:1046:GLN:HE21	1.86	0.41
1:E:43:ARG:CG	1:E:46:ARG:HH12	2.33	0.41
3:D:268:LEU:HD22	3:D:286:LEU:CD1	2.50	0.41
3:D:918:TYR:O	3:D:921:ASP:HB2	2.20	0.41
3:D:930:VAL:HG12	3:D:931:THR:N	2.34	0.41
1:B:121:VAL:CG2	1:B:257:LEU:HB3	2.50	0.41
1:E:25:HIS:ND1	1:E:26:PRO:HD2	2.35	0.41
3:D:218:ASN:HD22	3:D:218:ASN:C	2.23	0.41
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.21	0.41
3:A:24:ASP:OD1	3:A:24:ASP:C	2.59	0.41
3:A:153:ILE:HG13	3:A:154:VAL:N	2.36	0.41
3:A:338:GLU:OE2	3:A:409:TYR:HE2	2.03	0.41
3:A:887:ARG:HD2	3:A:887:ARG:HA	1.59	0.41
1:E:124:CYS:HA	1:E:125:PRO:HD3	1.68	0.41
3:D:398:GLN:O	3:D:399:HIS:O	2.38	0.41
3:D:888:ASN:ND2	3:D:888:ASN:N	2.68	0.41
2:F:118:VAL:HG23	2:F:164:LEU:HD21	2.03	0.41
3:D:146:TRP:N	3:D:147:PRO:CD	2.84	0.41
3:D:287:PHE:CE2	3:D:337:LEU:HD13	2.55	0.41
3:D:940:THR:O	3:D:944:SER:HB2	2.21	0.41
2:C:122:ASN:O	2:C:123:LYS:HB2	2.20	0.41
3:A:33:ASN:HD22	3:A:44:ARG:HE	1.69	0.41



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0		- <b>x</b>

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:290:THR:HG21	3:A:325:PHE:CZ	2.55	0.41
3:A:417:ARG:NH2	3:A:464:LEU:O	2.47	0.41
3:A:969:ASN:O	3:A:970:ASN:C	2.60	0.41
3:A:1009:PRO:O	3:A:1013:GLU:HG2	2.20	0.41
1:E:187:ASP:HB3	1:E:189:MET:CE	2.51	0.41
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.56	0.41
2:F:80:TYR:O	2:F:81:ILE:C	2.59	0.41
3:D:97:ASN:H	3:D:97:ASN:HD22	1.65	0.41
3:D:223:HIS:CE1	3:D:263:VAL:CG2	3.04	0.41
3:D:517:LEU:O	3:D:521:ILE:HG12	2.21	0.41
3:D:993:GLN:HG2	3:D:1033:LEU:HD13	2.03	0.41
3:D:1012:LYS:HE2	3:D:1012:LYS:HB3	1.85	0.41
1:B:58:TYR:HB3	1:B:197:TYR:CD1	2.56	0.41
2:C:54:THR:HG22	2:C:176:PHE:HD1	1.86	0.41
3:A:63:VAL:HA	3:A:76:LYS:CG	2.48	0.41
3:A:190:LYS:HB2	3:A:190:LYS:HE3	1.78	0.41
3:A:1034:PHE:C	3:A:1036:GLU:H	2.24	0.41
1:E:242:LEU:O	1:E:246:LEU:HB2	2.21	0.41
3:D:16:LEU:HD12	3:D:16:LEU:C	2.41	0.41
3:D:24:ASP:O	3:D:28:LEU:HB2	2.20	0.41
3:D:202:PHE:CE2	3:D:206:PHE:HD1	2.38	0.41
3:D:242:PHE:HB3	3:D:282:GLN:HG2	2.03	0.41
1:B:15:SER:HB2	8:B:546:HOH:O	2.20	0.40
3:A:467:LEU:HD23	3:A:467:LEU:N	2.36	0.40
3:A:962:LEU:O	3:A:962:LEU:HG	2.20	0.40
2:F:106:ARG:HD3	3:D:181:PHE:CD2	2.54	0.40
3:D:409:TYR:O	3:D:410:LEU:C	2.58	0.40
3:D:1009:PRO:O	3:D:1013:GLU:HG2	2.21	0.40
1:B:201:THR:HG22	1:B:204:ARG:HH12	1.85	0.40
1:E:245:VAL:HA	1:E:248:MET:HG3	2.03	0.40
3:D:231:ARG:HA	3:D:231:ARG:HD3	1.92	0.40
3:D:525:LEU:CD1	3:D:544:ILE:HD13	2.52	0.40
3:D:659:LEU:O	3:D:663:GLN:HG3	2.22	0.40
3:D:772:VAL:CG1	3:D:811:LEU:HD11	2.51	0.40
3:D:962:LEU:CB	3:D:964:PRO:HD3	2.51	0.40
3:D:975:GLN:HG2	3:D:998:VAL:HG12	2.02	0.40
1:B:35:TYR:CD2	1:B:35:TYR:O	2.75	0.40
1:B:41:SER:HB2	1:B:110:ASP:HB3	2.02	0.40
1:B:61:HIS:CG	1:B:94:LEU:HD13	2.55	0.40
1:B:124:CYS:HA	1:B:125:PRO:HD3	1.67	0.40
1:B:187:ASP:OD2	1:B:204:ARG:NH2	2.54	0.40



Atom 1	Atom 2	Interatomic	$\operatorname{Clash}$
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:A:419:LEU:HD23	3:A:420:MET:CE	2.52	0.40
3:A:422:SER:OG	3:A:479:LYS:HE3	2.21	0.40
3:A:549:GLY:HA3	8:A:1115:HOH:O	2.21	0.40
3:A:738:MET:C	3:A:740:THR:N	2.74	0.40
1:E:245:VAL:HA	1:E:248:MET:SD	2.61	0.40
3:D:179:PHE:HE2	3:D:198:MET:HE3	1.85	0.40
3:D:898:PHE:CE1	3:D:902:GLN:NE2	2.89	0.40
3:A:146:TRP:N	3:A:147:PRO:CD	2.84	0.40
3:D:222:VAL:O	3:D:226:LEU:HB2	2.21	0.40
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.86	0.40
3:A:289:LEU:HD12	3:A:289:LEU:N	2.36	0.40
3:A:465:THR:O	3:A:469:TYR:HB3	2.21	0.40
3:A:575:GLU:OE2	3:A:577:HIS:HB2	2.21	0.40
3:D:76:LYS:HE2	3:D:126:TYR:CZ	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	entiles
1	В	266/365~(73%)	241 (91%)	20 (8%)	5 (2%)	8	13
1	Е	277/365~(76%)	253 (91%)	16 (6%)	8 (3%)	4	6
2	С	170/216~(79%)	157 (92%)	11 (6%)	2(1%)	13	24
2	F	169/216~(78%)	157~(93%)	9(5%)	3(2%)	8	14
3	А	1042/1073~(97%)	945~(91%)	79 (8%)	18 (2%)	9	16
3	D	1045/1073~(97%)	952 (91%)	71 (7%)	22 (2%)	7	11
All	All	2969/3308~(90%)	2705 (91%)	206 (7%)	58 (2%)	8	12

All (58) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	160	ASN
1	В	216	GLU
1	В	351	PRO
2	С	169	ILE
3	А	123	GLU
3	А	390	ALA
3	А	963	ASN
1	Е	94	LEU
1	Ε	351	PRO
1	Ε	359	GLU
3	D	399	HIS
3	D	963	ASN
1	В	286	LEU
3	А	54	LYS
3	А	486	GLY
3	А	964	PRO
1	Ε	286	LEU
2	F	55	ASN
3	D	54	LYS
3	D	216	SER
3	D	486	GLY
3	D	490	SER
3	D	623	CYS
3	А	216	SER
3	А	217	GLN
3	А	490	SER
3	А	623	CYS
3	А	961	PRO
2	F	178	ALA
3	D	217	GLN
3	D	438	GLY
3	D	961	PRO
1	В	97	HIS
2	С	178	ALA
3	А	277	SER
3	A	281	GLU
3	A	743	PRO
1	E	358	MET
3	D	53	LEU
3	D	277	SER
3	D	487	THR
3	D	737[A]	GLU
3	D	737[B]	GLU



Mol	Chain	Res	Type
3	D	743	PRO
3	А	143	PRO
3	А	487	THR
3	D	143	PRO
3	D	281	GLU
3	D	679	LEU
3	А	55	GLU
3	А	955	GLU
1	Ε	52[A]	LYS
1	Е	52[B]	LYS
1	Ε	285	VAL
3	D	764	SER
3	D	955	GLU
3	D	111	ILE
2	F	81	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	249/327~(76%)	229~(92%)	20 (8%)	12 23
1	Е	257/327~(79%)	242 (94%)	15 (6%)	20 38
2	С	151/185~(82%)	138 (91%)	13 (9%)	10 20
2	F	150/185 (81%)	139 (93%)	11 (7%)	14 27
3	А	950/973~(98%)	889 (94%)	61 (6%)	17 33
3	D	953/973~(98%)	894 (94%)	59~(6%)	18 35
All	All	2710/2970~(91%)	2531 (93%)	179 (7%)	16 32

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	2	GLU
1	В	17[A]	ASP
1	В	17[B]	ASP



Mal	Chain	<b>P</b> oc	Turna
	D	nes	Type
1	B	35	TYR
1	B	111	VAL
1	В	120	ILE
1	B	129	ARG
1	В	156	LEU
1	В	189	MET
1	В	201	THR
1	В	222	THR
1	В	245	VAL
1	В	271	THR
1	В	277	LEU
1	В	284	ASP
1	В	285	VAL
1	В	352	ASP
1	В	353	HIS
1	В	357	LEU
1	В	360	ASN
2	С	15	LEU
2	С	21	THR
2	С	28	LYS
2	С	40	VAL
2	С	59	ILE
2	С	77	ASP
2	С	127	LYS
2	С	134	LYS
2	С	140	ARG
2	С	154	ASN
2	С	157	PHE
2	С	173	ASN
2	С	179	MET
3	А	18	ASP
3	A	23	LEU
3	A	24	ASP
3	A	25	ILE
3	A	60	TRP
3	A	62	ARG
3	A	71	GLN
3	A	80	LEU
3	A	81	GLN
3	A	96	ARG
3	A	97	ASN
3	A	119	CVS
0	11	113	010



Mol	Chain	Res	Type
3	А	146	TRP
3	А	150	ILE
3	A	165	GLN
3	A	189	VAL
3	A	192	LYS
3	А	194	LEU
3	А	200	ASN
3	А	205	ILE
3	А	208	LEU
3	А	218	ASN
3	А	229	LEU
3	А	257	VAL
3	А	263	VAL
3	А	292	MET
3	А	301	ASN
3	А	387	SER
3	А	393	LEU
3	А	394	LEU
3	А	401	ASP
3	А	426	LYS
3	А	436	ASP
3	А	443	GLU
3	А	481	GLN
3	А	525	LEU
3	А	530	GLN
3	А	535	ASP
3	А	578	ASP
3	А	620	THR
3	А	646	ASP
3	А	653	LEU
3	A	685	VAL
3	A	686	LYS
3	A	710	LEU
3	A	720	VAL
3	A	740	THR
3	A	746	ARG
3	А	749	ARG
3	А	781	LEU
3	А	807	ILE
3	A	875	LEU
3	А	882	PHE
3	A	887	ARG



Mol	Chain	Res	Type
3	А	888	ASN
3	А	907	GLU
3	А	968	VAL
3	A	999	THR
3	А	1008	ILE
3	А	1016	ARG
3	А	1043	ARG
1	Е	-2	LEU
1	Е	27	ARG
1	Е	35	TYR
1	Е	43	ARG
1	Е	47	LEU
1	Е	54	LYS
1	Е	56	LEU
1	Е	120	ILE
1	Е	126	VAL
1	Е	189	MET
1	Е	243	CYS
1	Е	245	VAL
1	Е	271	THR
1	Е	286	LEU
1	Е	353	HIS
2	F	13	LEU
2	F	15	LEU
2	F	34	GLU
2	F	55	ASN
2	F	59	ILE
2	F	119	LEU
2	F	134	LYS
2	F	140	ARG
2	F	154	ASN
2	F	157	PHE
2	F	177	VAL
3	D	14	ARG
3	D	18	ASP
3	D	25	ILE
3	D	37	HIS
3	D	60	TRP
3	D	80	LEU
3	D	81	GLN
3	D	96	ARG
3	D	97	ASN



Mol	Chain	Res	Type
3	D	122	LVS
<u></u>	D	1/16	TRP
<u>ु</u>	D	140	ILE
<u></u>		165	CLN
<u>-</u> 3	D	180	VAL
<u></u>		109	IVS
<u> </u>		192	LIS
<u></u>		200	ASN
<u></u>	D	200	CLN
<u>ე</u>	D	204	
<u></u>	D	$200 \\ 217$	CLN
<u>ა</u> ე	D	217	GLN
<u>ა</u> ე		218	ASN
<u>ა</u>		229	
<u>პ</u>		257	VAL
<u>პ</u>		203	VAL
3	D	301	ASN
3	D	312	
3	D	341	LEU
3	D	354	MET
3	D	401	ASP
3	D	426	LYS
3	D	436	ASP
3	D	447	ASP
3	D	525	LEU
3	D	535	ASP
3	D	578	ASP
3	D	646	ASP
3	D	653	LEU
3	D	655	GLU
3	D	686	LYS
3	D	710	LEU
3	D	724	LEU
3	D	727	ASN
3	D	740	THR
3	D	749	ARG
3	D	767	ASN
3	D	821	GLN
3	D	875	LEU
3	D	882	PHE
3	D	887	ARG
3	D	888	ASN
3	D	900	LEU



Conti	Continueu from previous puye								
Mol	Chain	$\operatorname{Res}$	Type						
3	D	999	THR						
3	D	1008	ILE						
3	D	1016	ARG						
3	D	1029	ASP						
3	D	1030	THR						
3	D	1031	SER						
3	D	1032	ASP						
3	D	1043	ARG						

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	В	19	ASN
1	В	51	GLN
1	В	61	HIS
1	В	101	GLN
1	В	200	GLN
1	В	261	HIS
1	В	353	HIS
2	С	30	HIS
2	С	105	HIS
2	С	145	GLN
2	С	154	ASN
2	С	156	ASN
3	А	30	ASN
3	А	33	ASN
3	А	37	HIS
3	А	56	HIS
3	А	71	GLN
3	А	97	ASN
3	А	145	HIS
3	А	166	ASN
3	А	204	GLN
3	А	210	GLN
3	А	215	ASN
3	A	218	ASN
3	А	293	GLN
3	А	296	GLN
3	A	321	ASN
3	А	352	HIS
3	A	437	GLN
3	А	456	ASN



Mol	Chain	Res	Type
3	А	483	GLN
3	А	558	HIS
3	А	574	HIS
3	А	577	HIS
3	А	626	GLN
3	А	631	HIS
3	А	704	HIS
3	А	775	ASN
3	А	791	ASN
3	А	821	GLN
3	А	853	GLN
3	А	888	ASN
3	А	924	GLN
3	А	963	ASN
3	А	969	ASN
3	А	970	ASN
3	А	988	HIS
3	А	993	GLN
3	А	1021	GLN
3	А	1046	GLN
3	А	1050	HIS
1	Е	19	ASN
1	Е	51	GLN
1	Е	61	HIS
1	Ε	101	GLN
1	Е	200	GLN
1	Е	209	HIS
1	Е	261	HIS
1	Е	263	GLN
1	Е	353	HIS
2	F	30	HIS
2	F	105	HIS
2	F	145	GLN
2	F	154	ASN
2	F	156	ASN
3	D	30	ASN
3	D	43	GLN
3	D	56	HIS
3	D	97	ASN
3	D	166	ASN
3	D	185	GLN
3	D	204	GLN



Mol	Chain	Res	Type
3	D	210	GLN
3	D	215	ASN
3	D	217	GLN
3	D	218	ASN
3	D	293	GLN
3	D	296	GLN
3	D	321	ASN
3	D	352	HIS
3	D	407	GLN
3	D	437	GLN
3	D	456	ASN
3	D	483	GLN
3	D	558	HIS
3	D	601	GLN
3	D	626	GLN
3	D	704	HIS
3	D	733	GLN
3	D	791	ASN
3	D	853	GLN
3	D	888	ASN
3	D	924	GLN
3	D	988	HIS
3	D	993	GLN
3	D	1021	GLN
3	D	1044	GLN
3	D	1046	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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	Trune	Chain	Dea Link		Bo	ond leng	$\mathbf{ths}$	B	ond ang	les
IVIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	GTP	С	217	-	26,34,34	0.98	1 (3%)	33,54,54	1.84	8 (24%)
5	GTP	F	217	-	26,34,34	0.97	1 (3%)	33,54,54	1.81	7 (21%)

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
5	GTP	С	217	-	-	2/18/38/38	0/3/3/3
5	GTP	F	217	-	-	2/18/38/38	0/3/3/3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	С	217	GTP	C6-N1	2.98	1.38	1.33
5	F	217	GTP	C6-N1	2.72	1.37	1.33

All (2) bond length outliers are listed below:

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
5	С	217	GTP	N3-C2-N1	-5.12	120.39	127.22
5	F	217	GTP	N3-C2-N1	-4.92	120.65	127.22
5	С	217	GTP	C2-N3-C4	3.99	119.91	115.36
5	F	217	GTP	C2-N3-C4	3.74	119.63	115.36
5	С	217	GTP	PA-O3A-PB	-3.65	120.32	132.83
5	F	217	GTP	PA-O3A-PB	-3.60	120.46	132.83
5	F	217	GTP	C5-C6-N1	-3.26	118.98	123.43
5	С	217	GTP	PB-O3B-PG	-3.13	122.09	132.83
5	С	217	GTP	C5-C6-N1	-3.11	119.17	123.43



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	F	217	GTP	PB-O3B-PG	-2.92	122.80	132.83
5	F	217	GTP	C6-N1-C2	2.82	120.42	115.93
5	С	217	GTP	C6-N1-C2	2.58	120.03	115.93
5	С	217	GTP	N2-C2-N1	2.24	120.73	117.25
5	F	217	GTP	C4-C5-N7	-2.17	107.14	109.40
5	С	217	GTP	O3G-PG-O3B	2.04	111.47	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	217	GTP	PG-O3B-PB-O1B
5	С	217	GTP	PG-O3B-PB-O1B
5	С	217	GTP	O4'-C4'-C5'-O5'
5	F	217	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	217	GTP	2	0
5	F	217	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









### 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	< <b>RSRZ</b> >	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	В	274/365~(75%)	0.23	8 (2%) 51 55	19, 36, 78, 112	3(1%)
1	Ε	279/365~(76%)	0.27	9 (3%) 47 51	19, 37, 85, 126	0
2	С	171/216~(79%)	0.21	2 (1%) 79 80	20,  43,  73,  99	0
2	F	171/216~(79%)	0.19	0 100 100	20, 42, 77, 99	0
3	А	1041/1073~(97%)	0.43	65 (6%) 20 21	14, 46, 100, 152	1 (0%)
3	D	1041/1073~(97%)	0.53	92 (8%) 10 10	16, 46, 107, 156	5 (0%)
All	All	2977/3308~(89%)	0.40	176 (5%) 22 23	14, 43, 96, 156	9 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	10.0
3	А	1053	GLN	9.0
3	D	967	PRO	8.0
3	D	1055	SER	7.8
3	D	19	PHE	7.7
3	D	966	ASN	7.3
3	D	1054	MET	7.1
3	D	115	SER	6.8
3	D	276	VAL	6.7
3	А	1029	ASP	6.7
3	А	70	SER	6.6
3	А	967	PRO	6.5
3	D	440	VAL	6.2
3	D	53	LEU	5.8
3	D	1052	LEU	5.6
3	D	119	CYS	5.5
3	А	397	SER	5.4
3	D	1025	5 PHE 5.	
3	D	965	GLY	5.2



Mol	Chain	Res	Type	RSRZ
3	D	964	PRO	5.2
3	А	1050	HIS	5.1
3	D	154 VAL		5.0
3	D	60	TRP	5.0
3	А	976	ASP	4.9
3	А	392	PRO	4.6
3	D	62	ARG	4.4
3	А	393	LEU	4.3
3	D	159	THR	4.3
3	А	968	VAL	4.2
3	D	70	SER	4.2
3	D	71	GLN	4.2
3	D	441	VAL	4.1
3	А	1030	THR	4.1
3	А	966	ASN	4.0
3	А	1052	LEU	4.0
3	D	54	LYS	3.9
3	А	1054	MET	3.9
3	D	22	LYS	3.9
3	D	395	SER	3.9
3	А	394	LEU	3.9
3	D	66	ILE	3.8
3	D	391	SER	3.8
3	D	120	VAL	3.8
3	D	310	ASN	3.8
3	D	436	ASP	3.7
3	D	213	MET	3.7
3	D	16	LEU	3.7
3	А	395	SER	3.7
3	D	44	ARG	3.7
1	Е	73	MET	3.7
3	A	1027	GLY	3.6
3	D	397	SER	3.6
3	D	1051	LYS	3.6
3	A	1033	LEU	3.6
3	D	37	HIS	3.6
2	С	178	ALA	3.5
3	D	1030	THR	3.5
3	A	1026	ALA	3.5
3	А	62	ARG	3.5
3	A	16	LEU	3.5
3	А	337	LEU	3.5



Continued from previous page...

 Mol
 Chain
 Res
 Type
 RSRZ

3         A         15         GLN         3.5           3         D         52         HIS         3.5           1         E         51         GLN         3.4           3         D         117         PRO         3.4           1         E         283         SER         3.4           3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         126         VAL         3.2           1         E         289         ALA         3.2           3         D         20         SER         3.1           3         D         20         SER         3.1           3         D         305         GLU         3.0           3         D         335         GLU         3.0	1,101	Onam	ICOD	-JPC	100102
3         D         52         HIS         3.5           1         E         51         GLN         3.4           3         D         117         PRO         3.4           1         E         283         SER         3.4           3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         A         120         VAL         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         126         VAL         3.2           1         E         289         ALA         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           1         B         350         SER         3.1           3         D         435         ASN         3.0           3         D         955         GLU         3.0 <tr< td=""><td>3</td><td>А</td><td>15</td><td>GLN</td><td>3.5</td></tr<>	3	А	15	GLN	3.5
1         E         51         GLN         3.4           3         D         117         PRO         3.4           1         E         283         SER         3.4           3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         A         114         SER         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.2           1         E         289         ALA         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           1         B         350         SER         3.1           3         D         20         SER         3.1           3         D         335         GLN         3.0           3         D         955         GLU         3.0 <t< td=""><td>3</td><td>D</td><td>52</td><td>HIS</td><td>3.5</td></t<>	3	D	52	HIS	3.5
3         D         117         PRO         3.4           1         E         283         SER         3.4           3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         A         114         SER         3.3           3         D         125         VAL         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           3         D         305         GLU         3.0           3         D         935         GLU         3.0           3         D         1050         HIS         3.0	1	Е	51	GLN	3.4
1         E         283         SER         3.4           3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         A         114         SER         3.3           3         D         125         VAL         3.3           3         D         336         LEU         3.2           1         E         289         ALA         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           3         D         20         SER         3.1           3         D         20         SER         3.1           3         D         350         SER         3.1           3         D         435         ASN         3.0           3         D         955         GLU         3.0           3         D         1050         HIS         3.0           3         D         983         LYS         2.9 <t< td=""><td>3</td><td>D</td><td>117</td><td>PRO</td><td>3.4</td></t<>	3	D	117	PRO	3.4
3         D         123         GLU         3.3           1         E         58         TYR         3.3           3         A         114         SER         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         326         LEU         3.2           1         E         289         ALA         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           1         B         350         SER         3.1           3         D         435         ASN         3.0           3         D         335         GLU         3.0           3         D         1050         HIS         3.0           3         D         1050         HIS         3.0           3         D         983         LYS         2.9           3         D         388         THR         2.9	1	Е	283	SER	3.4
1         E         58         TYR         3.3           3         A         120         VAL         3.3           3         D         125         VAL         3.3           3         D         125         VAL         3.3           3         D         336         LEU         3.2           1         E         289         ALA         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           3         D         20         SER         3.1           3         D         435         ASN         3.0           3         D         435         ASN         3.0           3         D         955         GLU         3.0           3         D         1050         HIS         3.0           3         D         964         ASP         3.0           3         D         983         LYS         2.9           3         D         3.0         3.0         3.0      <	3	D	123	GLU	3.3
3       A       120       VAL       3.3         3       D       125       VAL       3.3         3       D       336       LEU       3.2         1       E       289       ALA       3.2         3       A       276       VAL       3.2         3       A       276       VAL       3.2         3       D       1036       GLU       3.1         3       D       20       SER       3.1         1       B       350       SER       3.1         3       D       20       SER       3.1         3       D       355       GLN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       1050       HIS       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A	1	Е	58	TYR	3.3
3       A       114       SER       3.3         3       D       125       VAL       3.3         3       D       336       LEU       3.2         1       E       289       ALA       3.2         3       A       276       VAL       3.2         3       D       1036       GLU       3.1         3       D       20       SER       3.1         1       B       350       SER       3.1         3       D       20       SER       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       1050       HIS       3.0         3       D       1035       LEU       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       A       150       ILE       2.9         3       A <td< td=""><td>3</td><td>А</td><td>120</td><td>VAL</td><td>3.3</td></td<>	3	А	120	VAL	3.3
3         D         125         VAL         3.3           3         D         336         LEU         3.2           1         E         289         ALA         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           1         B         350         SER         3.1           3         A         399         HIS         3.1           3         D         435         ASN         3.0           3         D         335         GLN         3.0           3         D         955         GLU         3.0           3         D         1050         HIS         3.0           3         D         64         ASP         3.0           3         D         983         LYS         2.9           3         D         288         THR         2.9           3         A         150         ILE         2.9           3         A         258         PRO         2.8	3	А	114	SER	3.3
3         D         336         LEU         3.2           1         E         289         ALA         3.2           3         A         276         VAL         3.2           3         D         1036         GLU         3.1           3         D         20         SER         3.1           1         B         350         SER         3.1           3         A         399         HIS         3.1           3         D         435         ASN         3.0           3         D         335         GLN         3.0           3         D         955         GLU         3.0           3         D         1050         HIS         3.0           3         D         1050         HIS         3.0           3         D         983         LYS         2.9           3         D         288         THR         2.9           3         D         399         HIS         2.9           3         A         258         PRO         2.8           3         D         996         LEU         2.9	3	D	125	VAL	3.3
1       E       289       ALA       3.2         3       A       276       VAL       3.2         3       D       1036       GLU       3.1         3       D       20       SER       3.1         1       B       350       SER       3.1         3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       435       ASN       3.0         3       D       955       GLU       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       258       ILE       2.9         3       A       258       PRO       2.8         3       D       18	3	D	336	LEU	3.2
3       A       276       VAL       3.2         3       D       1036       GLU       3.1         3       D       20       SER       3.1         1       B       350       SER       3.1         3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       A       150       ILE       2.9         3       A       258       PRO       2.8         3       D       186       ILE       2.8         3       D	1	Е	289	ALA	3.2
3       D       1036       GLU       3.1         3       D       20       SER       3.1         1       B       350       SER       3.1         3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       D       18	3	А	276	VAL	3.2
3       D       20       SER       3.1         1       B       350       SER       3.1         3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       983       LYS       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       D       186       ILE       2.8         3       D       186       ILE       2.8         3       A       105<	3	D	1036	GLU	3.1
1       B       350       SER       3.1         3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       D       996       LEU       2.9         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         3       D       3	3	D	20	SER	3.1
3       A       399       HIS       3.1         3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         3       D       337       LEU       2.7         3       A       939	1	В	350	SER	3.1
3       D       435       ASN       3.0         3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       288       THR       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       D       996       LEU       2.9         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         3       D       337       LEU       2.7         3       A       105<	3	А	399	HIS	3.1
3       D       335       GLN       3.0         3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       D       64       ASP       3.0         3       D       983       LYS       2.9         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       D       186       ILE       2.8         3       D       186       ILE       2.8         3       D       337       LEU       2.7         3       A       939       LEU       2.7         3       D       313 </td <td>3</td> <td>D</td> <td>435</td> <td>ASN</td> <td>3.0</td>	3	D	435	ASN	3.0
3       D       955       GLU       3.0         3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       A       1035       LEU       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       D       93	3	D	335	GLN	3.0
3       D       1050       HIS       3.0         3       D       64       ASP       3.0         3       A       1035       LEU       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       D       3	3	D	955	GLU	3.0
3         D         64         ASP         3.0           3         A         1035         LEU         3.0           3         D         983         LYS         2.9           3         D         288         THR         2.9           3         D         288         THR         2.9           3         D         399         HIS         2.9           3         A         150         ILE         2.9           3         A         25         ILE         2.9           3         A         25         ILE         2.9           3         A         25         ILE         2.9           3         A         258         PRO         2.8           3         A         1028         GLU         2.8           3         D         186         ILE         2.8           1         B         239         PRO         2.8           3         D         337         LEU         2.8           3         A         105         TYR         2.7           3         A         939         LEU         2.7 <t< td=""><td>3</td><td>D</td><td>1050</td><td>HIS</td><td>3.0</td></t<>	3	D	1050	HIS	3.0
3       A       1035       LEU       3.0         3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       313       ASP       2.7         3       D       4	3	D	64	ASP	3.0
3       D       983       LYS       2.9         3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       PRO       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       313       ASP       2.7         3       D       487 <td>3</td> <td>А</td> <td>1035</td> <td>LEU</td> <td>3.0</td>	3	А	1035	LEU	3.0
3       D       288       THR       2.9         3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       48	3	D	983	LYS	2.9
3       D       399       HIS       2.9         3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       A       25       ILE       2.9         3       D       996       LEU       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       7	3	D	288	THR	2.9
3       A       150       ILE       2.9         3       A       25       ILE       2.9         3       D       996       LEU       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       71       GLN       2.6	3	D	399	HIS	2.9
3       A       25       ILE       2.9         3       D       996       LEU       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       313       ASP       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       71       GLN       2.6	3	А	150	ILE	2.9
3       D       996       LEU       2.9         3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       71       GLN       2.6	3	А	25	ILE	2.9
3       A       258       PRO       2.8         3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       71       GLN       2.6	3	D	996	LEU	2.9
3       A       1028       GLU       2.8         3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         1       B       358       MET       2.7         3       A       71       GLN       2.6	3	А	258	PRO	2.8
3       D       186       ILE       2.8         1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       313       ASP       2.7         3       D       313       ASP       2.7         3       D       313       MSP       2.7         3       D       313       ASP       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         3       A       71       GLN       2.6	3	А	1028	GLU	2.8
1       B       239       PRO       2.8         1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       313       ASP       2.7         3       D       313       ASP       2.7         3       D       313       MSP       2.7         3       D       313       ASP       2.7         3       A       71       GLN       2.7         3       A       71       GLN       2.6	3	D	186	ILE	2.8
1       B       349       HIS       2.8         3       D       337       LEU       2.8         3       A       105       TYR       2.7         3       A       939       LEU       2.7         3       D       98       GLN       2.7         3       D       98       GLN       2.7         3       D       487       THR       2.7         3       D       487       THR       2.7         1       B       358       MET       2.7         3       A       71       GLN       2.6	1	В	239	PRO	2.8
3         D         337         LEU         2.8           3         A         105         TYR         2.7           3         A         939         LEU         2.7           3         D         98         GLN         2.7           3         D         98         GLN         2.7           3         D         313         ASP         2.7           3         D         313         ASP         2.7           3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	1	В	349	HIS	2.8
3         A         105         TYR         2.7           3         A         939         LEU         2.7           3         D         98         GLN         2.7           3         D         313         ASP         2.7           3         D         313         ASP         2.7           3         D         313         ASP         2.7           3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	3	D	337	LEU	2.8
3         A         939         LEU         2.7           3         D         98         GLN         2.7           3         D         313         ASP         2.7           3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	3	А	105	TYR	2.7
3         D         98         GLN         2.7           3         D         313         ASP         2.7           3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	3	А	939	LEU	2.7
3         D         313         ASP         2.7           3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	3	D	98	GLN	2.7
3         D         487         THR         2.7           1         B         358         MET         2.7           3         A         71         GLN         2.6	3	D	313	ASP	2.7
1         B         358         MET         2.7           3         A         71         GLN         2.6	3	D	487	THR	2.7
3 A 71 GLN 2.6	1	В	358	MET	2.7
	3	А	71	GLN	2.6



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Mol	Chain	Res	Type	RSRZ			
3	D	1027	GLY	2.6			
3	D	162	SER	2.6			
3	D	51	THR	2.6			
3	D	434	GLU	2.6			
3	А	22	LYS	2.6			
3	А	42	GLN	2.6			
3	А	63	VAL	2.5			
3	А	492	LYS	2.5			
3	А	955	GLU	2.5			
3	А	163	LEU	2.5			
3	А	284	GLU	2.5			
3	D	27	LEU	2.5			
3	А	43	GLN	2.5			
3	А	316	GLN	2.5			
3	А	110	ILE	2.5			
1	Ε	349	HIS	2.4			
3	D	939	LEU	2.4			
1	В	351	PRO	2.4			
3	D	230	LEU	2.4			
3	А	275	SER	2.4			
3	А	37	HIS	2.4			
3	D	142	TRP	2.4			
3	А	167	ASN	2.4			
3	А	400	PHE	2.4			
3	D	1018	PHE	2.3			
3	D	604	VAL	2.3			
3	D	1008	ILE	2.3			
3	А	199	CYS	2.3			
3	D	277	SER	2.3			
3	D	1004	LEU	2.3			
1	Е	97[A]	HIS	2.3			
1	Е	55	ARG	2.3			
3	D	968	VAL	2.3			
1	В	96	LYS	2.3			
3	А	485	ASN	2.3			
3	D	396	GLY	2.3			
3	А	1055	SER	2.2			
3	D	446	LYS	2.2			
3	D	271	ILE	2.2			
3	D	17	LEU	2.2			
3	D	121	GLU	2.2			
3	А	119	CYS	2.2			

119CYS2.2Continued on next page...



Mol	Chain	Res	Type	RSRZ
1	В	246	LEU	2.2
3	А	208	LEU	2.2
3	А	182	SER	2.2
3	D	118	THR	2.2
3	D	1019	LEU	2.2
3	А	280	GLU	2.2
3	А	995	LYS	2.2
3	D	346	ALA	2.2
3	D	962	LEU	2.2
3	А	14	ARG	2.1
3	D	989	LEU	2.1
3	D	1047	GLU	2.1
3	D	206	PHE	2.1
3	D	253	LYS	2.1
1	В	54	LYS	2.1
3	А	396	GLY	2.1
3	D	437	GLN	2.1
3	А	1038	ARG	2.1
2	С	59	ILE	2.1
3	А	23	LEU	2.1
3	D	344	ARG	2.1
3	А	98	GLN	2.1
3	D	245	LYS	2.1
3	А	436	ASP	2.0
3	D	215	ASN	2.0
1	Е	282	VAL	2.0
3	А	1044	GLN	2.0
3	D	969	ASN	2.0
3	А	252	TYR	2.0
3	D	134	LEU	2.0
3	D	275	SER	2.0

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### 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	MG	С	218	1/1	0.77	0.17	40,40,40,40	0
4	NA	Е	361	1/1	0.83	0.19	64,64,64,64	0
4	NA	В	361	1/1	0.92	0.18	34,34,34,34	0
6	MG	F	218	1/1	0.95	0.15	33,33,33,33	0
7	CL	Е	362	1/1	0.95	0.11	49,49,49,49	0
5	GTP	С	217	32/32	0.97	0.14	13,27,39,52	0
5	GTP	F	217	32/32	0.98	0.15	14,27,40,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers (i)

There are no such residues in this entry.

