



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2021 – 04:09 PM JST

PDB ID : 7EFL  
Title : Crystal structure of the gastric proton pump K791S in (BYK)E2BeF state  
Authors : Abe, K.; Yamamoto, K.; Irie, K.  
Deposited on : 2021-03-22  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

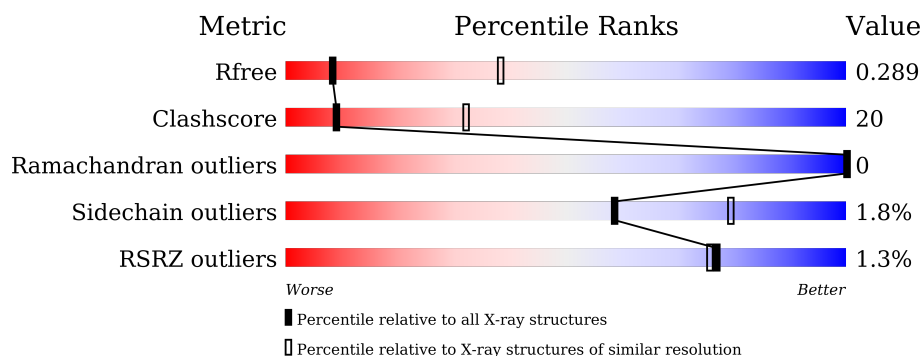
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	987	<div> <div></div> <div>63%</div> <div>36%</div> <div>.</div> </div>
2	B	255	<div> <div></div> <div>65%</div> <div>33%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	BFD	A	385	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	987	Total	Be	C	F	N	O	S	0	0	0
			7660	1	4887	3	1291	1424	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP A0A5G2QYH2
A	791	SER	LYS	engineered mutation	UNP A0A5G2QYH2
A	1005	SER	GLY	conflict	UNP A0A5G2QYH2

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			2037	1326	334	366	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	MET	-	initiating methionine	UNP P18434

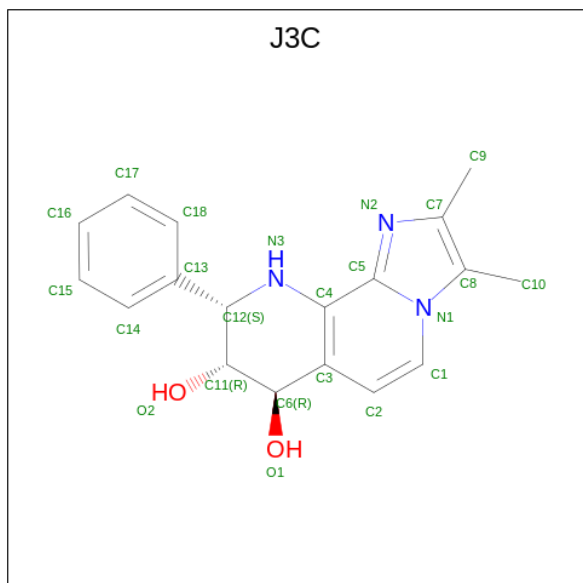
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Rb	0	0
			3	3		
4	B	1	Total	Rb	0	0
			1	1		

- Molecule 5 is (7R,8R,9S)-2,3-dimethyl-9-phenyl-7,8,9,10-tetrahydroimidazo[1,2-h][1,7]naphthyridine-7,8-diol (three-letter code: J3C) (formula:  $C_{18}H_{19}N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	18	3	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

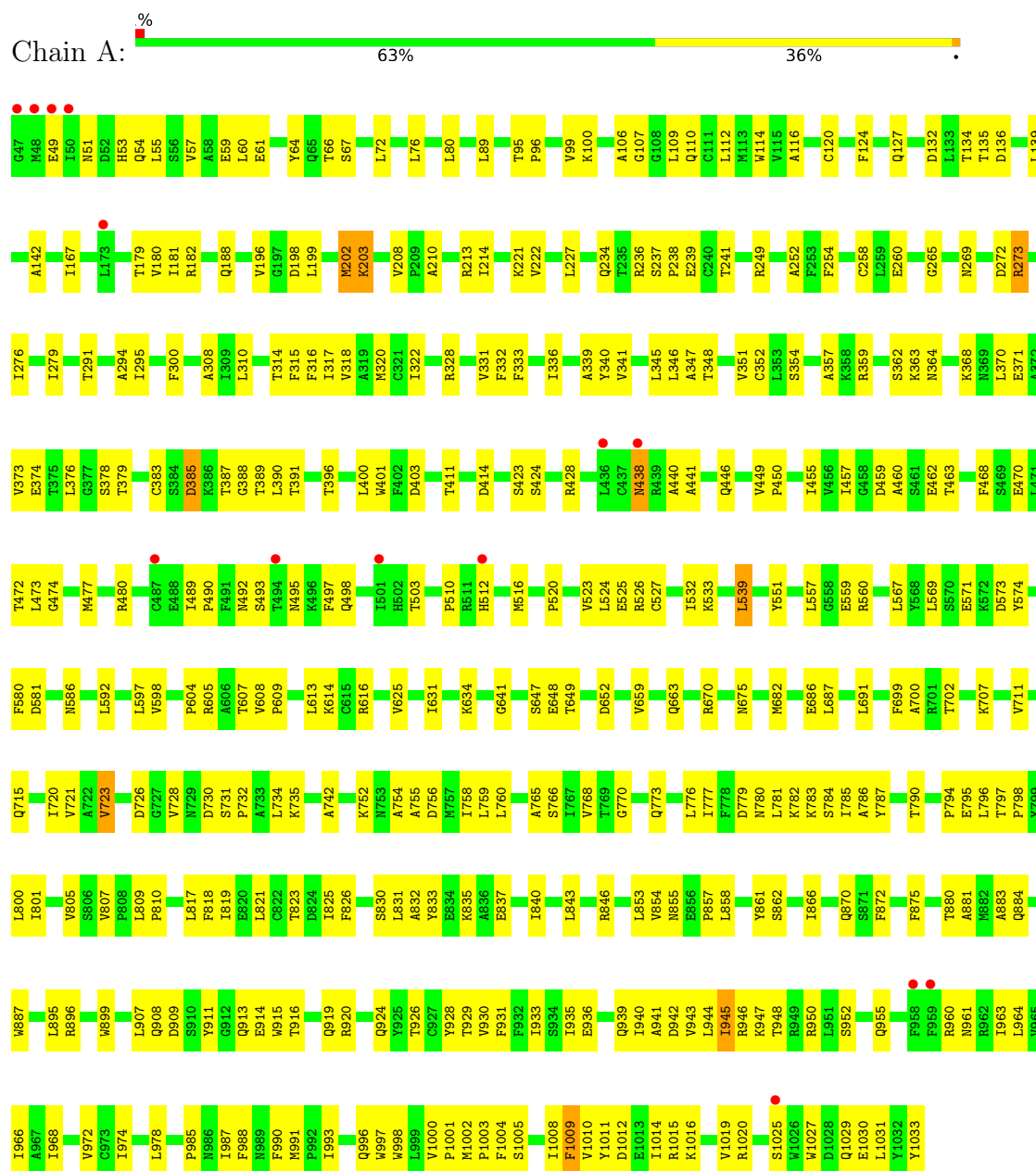
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		

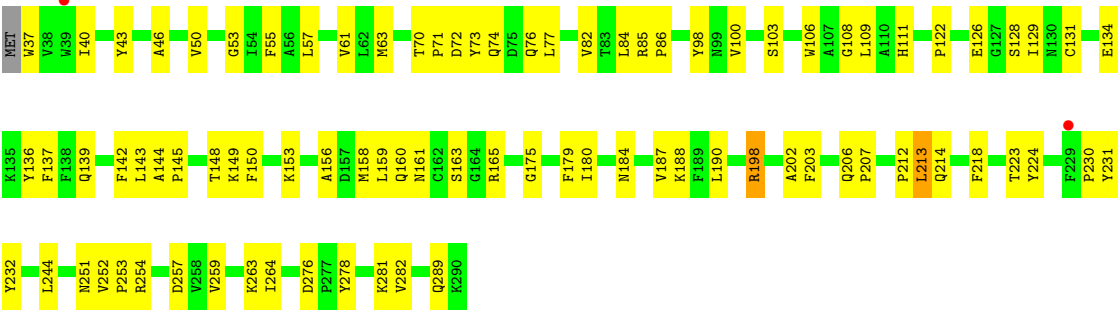
### 3 Residue-property plots

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: Sodium/potassium-transporting ATPase subunit alpha



- Molecule 2: Potassium-transporting ATPase subunit beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.97Å 104.97Å 369.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.29 – 3.40 48.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.29-3.40) 87.8 (48.29-3.10)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.230 , 0.289 0.230 , 0.289	Depositor DCC
$R_{free}$ test set	1922 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.070 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: J3C, MG, BFD, RB, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	1/7805 (0.0%)	0.75	2/10601 (0.0%)
2	B	0.52	0/2104	0.68	0/2864
All	All	0.57	1/9909 (0.0%)	0.74	2/13465 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	723	VAL	CB-CG2	-5.18	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	MET	CG-SD-CE	-9.23	85.43	100.20
1	A	539	LEU	CA-CB-CG	6.38	129.96	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7660	0	7677	319	0
2	B	2037	0	1975	86	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	1	0	0	0	0
5	A	23	0	0	0	0
6	B	28	0	26	0	0
7	A	3	0	0	0	0
All	All	9756	0	9678	391	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 20.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:ASP:CA	1:A:945:ILE:CD1	1.91	1.46
1:A:942:ASP:HA	1:A:945:ILE:CD1	1.01	1.45
1:A:942:ASP:CA	1:A:945:ILE:HD12	1.49	1.32
1:A:942:ASP:CA	1:A:945:ILE:HD11	1.67	1.08
1:A:942:ASP:C	1:A:945:ILE:HD12	1.75	1.05
1:A:941:ALA:O	1:A:945:ILE:HG13	1.59	1.03
1:A:941:ALA:O	1:A:945:ILE:CG1	2.08	1.01
1:A:942:ASP:HA	1:A:945:ILE:HD11	1.03	0.98
1:A:909:ASP:HB3	1:A:915:TRP:HH2	1.28	0.96
1:A:607:THR:HG21	1:A:765:ALA:HB2	1.48	0.91
2:B:144:ALA:HB3	2:B:148:THR:HG23	1.50	0.90
1:A:942:ASP:HA	1:A:945:ILE:HD12	0.91	0.90
1:A:942:ASP:O	1:A:945:ILE:HD12	1.73	0.89
1:A:915:TRP:CD1	2:B:77:LEU:HD21	2.08	0.89
1:A:941:ALA:C	1:A:945:ILE:HD11	1.93	0.88
1:A:942:ASP:N	1:A:945:ILE:HD11	1.89	0.86
1:A:941:ALA:O	1:A:945:ILE:CD1	2.23	0.86
1:A:915:TRP:HD1	2:B:77:LEU:HD21	1.40	0.86
1:A:942:ASP:HA	1:A:945:ILE:HD13	1.51	0.85
2:B:203:PHE:HE1	2:B:213:LEU:HB3	1.44	0.83
1:A:941:ALA:O	1:A:945:ILE:HD11	1.80	0.82
2:B:203:PHE:CE1	2:B:213:LEU:HB3	2.15	0.81
1:A:909:ASP:HB3	1:A:915:TRP:CH2	2.15	0.81
1:A:516:MET:HE1	1:A:523:VAL:HA	1.66	0.78
1:A:320:MET:HA	1:A:320:MET:HE2	1.68	0.75
1:A:723:VAL:HG23	1:A:734:LEU:HD23	1.68	0.75
1:A:798:PRO:HB3	1:A:810:PRO:HG2	1.68	0.74
1:A:913:GLN:HE21	2:B:187:VAL:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:TYR:HH	2:B:43:TYR:HH	1.34	0.72
1:A:1016:LYS:HA	1:A:1019:VAL:HG12	1.72	0.72
2:B:198:ARG:HB3	2:B:223:THR:HG22	1.72	0.72
1:A:167:ILE:HD13	1:A:758:ILE:HD12	1.71	0.72
1:A:438:ASN:O	1:A:480:ARG:NH1	2.23	0.71
1:A:260:GLU:HB3	1:A:459:ASP:HB3	1.70	0.71
1:A:222:VAL:HG23	1:A:258:CYS:HA	1.73	0.70
1:A:308:ALA:HA	1:A:340:TYR:CD2	2.26	0.70
1:A:276:ILE:HD13	1:A:728:VAL:HG21	1.74	0.70
1:A:109:LEU:HB2	1:A:346:LEU:HD13	1.73	0.70
1:A:359:ARG:NH1	1:A:773:GLN:OE1	2.22	0.69
1:A:468:PHE:O	1:A:472:THR:HG22	1.91	0.69
1:A:786:ALA:HB2	1:A:858:LEU:HD11	1.75	0.68
1:A:854:VAL:HA	1:A:858:LEU:HD23	1.75	0.68
1:A:909:ASP:OD1	1:A:913:GLN:N	2.28	0.67
1:A:659:VAL:HG12	1:A:663:GLN:OE1	1.95	0.67
1:A:328:ARG:HA	1:A:331:VAL:HG12	1.77	0.67
1:A:391:THR:HA	1:A:604:PRO:HA	1.78	0.66
1:A:1004:PHE:O	1:A:1008:ILE:HG13	1.95	0.66
1:A:300:PHE:CD1	1:A:854:VAL:HG21	2.32	0.65
1:A:446:GLN:OE1	1:A:455:ILE:HD12	1.97	0.65
1:A:357:ALA:HB2	1:A:373:VAL:HG21	1.78	0.65
1:A:765:ALA:O	1:A:768:VAL:HG12	1.97	0.65
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.32	0.64
1:A:985:PRO:HB3	1:A:991:MET:HG2	1.79	0.64
1:A:707:LYS:O	1:A:711:VAL:HG23	1.98	0.64
1:A:291:THR:HG23	1:A:294:ALA:H	1.63	0.64
1:A:880:THR:HG22	1:A:997:TRP:HE1	1.64	0.64
1:A:887:TRP:CZ2	1:A:915:TRP:CZ3	2.85	0.64
1:A:884:GLN:O	2:B:72:ASP:HB3	1.97	0.63
1:A:916:THR:O	1:A:920:ARG:HG3	1.97	0.63
1:A:777:ILE:O	1:A:781:LEU:N	2.26	0.63
2:B:139:GLN:NE2	2:B:150:PHE:O	2.31	0.63
1:A:359:ARG:O	1:A:362:SER:OG	2.17	0.62
1:A:723:VAL:CG2	1:A:734:LEU:HA	2.30	0.62
2:B:122:PRO:O	2:B:126:GLU:HG3	2.00	0.62
1:A:1010:VAL:O	1:A:1014:ILE:HG22	2.00	0.62
1:A:300:PHE:HD1	1:A:854:VAL:HG21	1.64	0.62
1:A:385:BFD:O	1:A:389:THR:OG1	2.18	0.61
2:B:143:LEU:HB2	2:B:150:PHE:CE2	2.36	0.61
1:A:825:ILE:N	1:A:825:ILE:HD12	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:THR:HG22	1:A:993:ILE:HD11	1.83	0.61
1:A:723:VAL:HG21	1:A:734:LEU:HA	1.83	0.61
1:A:908:GLN:HA	1:A:913:GLN:O	2.00	0.61
2:B:143:LEU:N	2:B:148:THR:O	2.33	0.61
1:A:825:ILE:HD12	1:A:825:ILE:H	1.67	0.60
1:A:107:GLY:O	1:A:110:GLN:HG2	2.01	0.60
1:A:996:GLN:NE2	2:B:73:TYR:OH	2.35	0.60
2:B:202:ALA:HA	2:B:213:LEU:CD2	2.32	0.60
1:A:374:GLU:OE2	1:A:378:SER:OG	2.18	0.59
1:A:210:ALA:O	1:A:254:PHE:HA	2.03	0.59
1:A:76:LEU:HD23	1:A:80:LEU:HG	1.84	0.59
1:A:213:ARG:NH1	1:A:214:ILE:O	2.36	0.59
1:A:276:ILE:O	1:A:279:ILE:HG22	2.03	0.59
1:A:926:THR:O	1:A:930:VAL:HG12	2.03	0.58
2:B:136:TYR:HE2	2:B:190:LEU:HD22	1.67	0.58
1:A:53:HIS:CD2	1:A:54:GLN:HG3	2.38	0.58
1:A:933:ILE:HD12	1:A:993:ILE:HD12	1.84	0.58
2:B:84:LEU:O	2:B:85:ARG:HD3	2.03	0.58
1:A:57:VAL:O	1:A:61:GLU:HG2	2.02	0.58
1:A:819:ILE:HA	1:A:823:THR:HG22	1.86	0.58
1:A:835:LYS:HB2	1:A:960:ARG:HH21	1.68	0.58
1:A:682:MET:HB3	1:A:686:GLU:HB2	1.84	0.58
1:A:1019:VAL:HB	1:A:1027:TRP:HD1	1.68	0.58
2:B:57:LEU:O	2:B:61:VAL:HG23	2.04	0.58
1:A:818:PHE:HD2	1:A:978:LEU:HD11	1.69	0.58
1:A:120:CYS:HB2	1:A:142:ALA:HB2	1.85	0.58
1:A:182:ARG:NH2	1:A:198:ASP:OD2	2.32	0.57
1:A:907:LEU:O	1:A:914:GLU:HA	2.04	0.57
1:A:438:ASN:HD21	1:A:462:GLU:HB3	1.69	0.57
1:A:911:TYR:CE2	2:B:71:PRO:HA	2.39	0.57
1:A:89:LEU:HD11	1:A:254:PHE:HE2	1.70	0.57
1:A:202:MET:HE2	1:A:258:CYS:HB2	1.86	0.57
1:A:783:LYS:NZ	1:A:837:GLU:OE2	2.28	0.57
1:A:236:ARG:HH21	1:A:249:ARG:HA	1.68	0.57
1:A:376:LEU:HD12	1:A:770:GLY:HA3	1.87	0.56
2:B:156:ALA:O	2:B:163:SER:OG	2.23	0.56
1:A:308:ALA:HA	1:A:340:TYR:HD2	1.67	0.56
1:A:916:THR:HG21	2:B:276:ASP:OD2	2.05	0.56
2:B:63:MET:HE2	2:B:63:MET:HA	1.88	0.56
1:A:273:ARG:H	1:A:273:ARG:HD2	1.69	0.56
2:B:136:TYR:CE2	2:B:190:LEU:HD22	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ILE:HG21	2:B:244:LEU:HD22	1.88	0.56
1:A:861:TYR:CZ	1:A:866:ILE:HD11	2.41	0.56
1:A:495:ASN:HB3	1:A:497:PHE:CE2	2.41	0.55
2:B:187:VAL:HG22	2:B:231:TYR:HD2	1.71	0.55
2:B:202:ALA:HA	2:B:213:LEU:HD22	1.88	0.55
1:A:735:LYS:HG3	1:A:754:ALA:HB1	1.89	0.55
2:B:129:ILE:O	2:B:153:LYS:HG3	2.06	0.55
1:A:742:ALA:HB3	1:A:758:ILE:HG12	1.88	0.55
1:A:835:LYS:HB2	1:A:960:ARG:NH2	2.22	0.55
1:A:503:THR:HG22	1:A:512:HIS:CE1	2.42	0.55
1:A:569:LEU:HB3	1:A:574:TYR:CD2	2.42	0.54
2:B:206:GLN:N	2:B:207:PRO:HD3	2.23	0.54
1:A:926:THR:N	1:A:991:MET:HE1	2.22	0.54
1:A:866:ILE:HD12	1:A:866:ILE:N	2.22	0.54
1:A:179:THR:HG22	1:A:188:GLN:OE1	2.08	0.54
2:B:160:GLN:H	2:B:218:PHE:HB3	1.73	0.54
1:A:526:ARG:O	1:A:592:LEU:HB2	2.08	0.54
2:B:82:VAL:HG23	2:B:282:VAL:HB	1.90	0.54
2:B:188:LYS:HA	2:B:230:PRO:HB2	1.90	0.54
1:A:759:LEU:HD22	1:A:766:SER:HB2	1.90	0.54
2:B:100:VAL:HG22	2:B:289:GLN:O	2.08	0.54
1:A:385:BFD:HB2	1:A:389:THR:HG21	1.90	0.53
1:A:116:ALA:HB2	1:A:341:VAL:HG21	1.89	0.53
2:B:137:PHE:HE2	2:B:139:GLN:HE21	1.57	0.53
2:B:144:ALA:CB	2:B:148:THR:HG23	2.30	0.53
1:A:872:PHE:HD2	2:B:55:PHE:HB2	1.73	0.53
1:A:401:TRP:HB3	1:A:597:LEU:HB2	1.90	0.53
1:A:794:PRO:HG3	1:A:870:GLN:HB2	1.90	0.53
2:B:71:PRO:HD3	2:B:187:VAL:HB	1.90	0.53
1:A:291:THR:HG21	1:A:371:GLU:HB3	1.90	0.53
1:A:616:ARG:NH1	1:A:641:GLY:O	2.42	0.53
1:A:787:TYR:HB2	1:A:946:ARG:HG3	1.91	0.53
1:A:120:CYS:CB	1:A:142:ALA:HB2	2.39	0.52
1:A:490:PRO:HA	1:A:498:GLN:HG2	1.90	0.52
1:A:1002:MET:N	1:A:1003:PRO:HD2	2.25	0.52
1:A:929:THR:OG1	1:A:990:PHE:HA	2.08	0.52
1:A:379:THR:HG23	1:A:720:ILE:O	2.10	0.52
1:A:880:THR:HG22	1:A:997:TRP:NE1	2.24	0.52
1:A:819:ILE:HA	1:A:823:THR:CG2	2.40	0.51
2:B:175:GLY:HA3	2:B:254:ARG:NH2	2.26	0.51
1:A:383:CYS:HB2	1:A:723:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:PRO:HB3	1:A:991:MET:CG	2.40	0.51
1:A:441:ALA:O	1:A:457:ILE:HD12	2.09	0.51
1:A:941:ALA:HB2	1:A:1005:SER:HB2	1.91	0.51
1:A:731:SER:OG	1:A:732:PRO:HD3	2.11	0.51
1:A:779:ASP:O	1:A:783:LYS:HG3	2.11	0.51
1:A:1016:LYS:HA	1:A:1019:VAL:CG1	2.41	0.51
1:A:854:VAL:HG23	1:A:854:VAL:O	2.11	0.51
1:A:460:ALA:HA	1:A:463:THR:HB	1.93	0.51
1:A:127:GLN:HE21	1:A:331:VAL:HG21	1.76	0.50
1:A:132:ASP:O	1:A:135:THR:OG1	2.27	0.50
1:A:260:GLU:HB3	1:A:459:ASP:CB	2.41	0.50
1:A:855:ASN:HB2	1:A:857:PRO:HD2	1.92	0.50
1:A:944:LEU:HD21	1:A:968:ILE:CD1	2.41	0.50
1:A:944:LEU:HD21	1:A:968:ILE:HD11	1.92	0.50
1:A:809:LEU:HG	1:A:928:TYR:HE1	1.77	0.50
1:A:459:ASP:O	1:A:463:THR:N	2.41	0.50
1:A:332:PHE:O	1:A:336:ILE:HG13	2.12	0.50
1:A:315:PHE:CD2	1:A:800:LEU:HD22	2.47	0.50
2:B:86:PRO:HD2	2:B:179:PHE:CD1	2.47	0.50
1:A:945:ILE:HG22	1:A:1012:ASP:OD2	2.12	0.49
1:A:55:LEU:HD22	1:A:59:GLU:HB3	1.94	0.49
2:B:103:SER:HA	2:B:106:TRP:CE2	2.47	0.49
1:A:963:ILE:HA	1:A:966:ILE:HG22	1.93	0.49
1:A:880:THR:HG23	1:A:884:GLN:HE21	1.77	0.49
1:A:315:PHE:CZ	1:A:800:LEU:HD13	2.47	0.49
1:A:472:THR:HG23	1:A:473:LEU:H	1.78	0.49
1:A:895:LEU:HD23	1:A:899:TRP:HB2	1.94	0.49
1:A:520:PRO:HG2	1:A:551:TYR:CE1	2.47	0.48
2:B:159:LEU:O	2:B:163:SER:OG	2.21	0.48
1:A:440:ALA:O	1:A:480:ARG:NH2	2.35	0.48
1:A:492:ASN:OD1	1:A:493:SER:N	2.44	0.48
1:A:993:ILE:CG2	1:A:997:TRP:HE3	2.26	0.48
2:B:142:PHE:HA	2:B:149:LYS:HG2	1.95	0.48
1:A:339:ALA:CB	1:A:796:LEU:HD13	2.44	0.48
2:B:53:GLY:O	2:B:57:LEU:HG	2.13	0.48
1:A:347:ALA:O	1:A:351:VAL:HG22	2.14	0.48
1:A:510:PRO:HG2	1:A:571:GLU:HG3	1.95	0.48
1:A:1015:ARG:NH2	1:A:1033:TYR:HE1	2.10	0.48
1:A:64:TYR:HE2	1:A:196:VAL:CG1	2.27	0.48
2:B:76:GLN:C	2:B:77:LEU:HD23	2.34	0.48
1:A:682:MET:HB3	1:A:686:GLU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLU:O	1:A:474:GLY:HA2	2.14	0.47
1:A:675:ASN:HA	1:A:700:ALA:O	2.13	0.47
1:A:887:TRP:CZ2	1:A:915:TRP:CH2	3.02	0.47
1:A:210:ALA:HA	1:A:254:PHE:HD1	1.78	0.47
1:A:790:THR:HG22	1:A:862:SER:HB3	1.95	0.47
2:B:190:LEU:HD21	2:B:230:PRO:HG3	1.96	0.47
1:A:89:LEU:N	1:A:89:LEU:HD12	2.30	0.47
1:A:527:CYS:HA	1:A:592:LEU:O	2.14	0.47
1:A:794:PRO:HB2	1:A:935:ILE:CD1	2.44	0.47
1:A:823:THR:HB	1:A:974:ILE:HD11	1.97	0.47
1:A:947:LYS:NZ	1:A:960:ARG:HB3	2.28	0.47
1:A:64:TYR:CE2	1:A:196:VAL:HG12	2.50	0.47
1:A:784:SER:HA	1:A:831:LEU:HD13	1.95	0.47
2:B:128:SER:OG	2:B:153:LYS:HG2	2.14	0.46
1:A:106:ALA:O	1:A:110:GLN:HG3	2.14	0.46
1:A:203:LYS:HB3	1:A:203:LYS:HE2	1.51	0.46
1:A:730:ASP:O	1:A:731:SER:C	2.53	0.46
2:B:212:PRO:O	2:B:251:ASN:ND2	2.48	0.46
2:B:187:VAL:HG13	2:B:232:TYR:HA	1.97	0.46
1:A:400:LEU:HD23	1:A:598:VAL:HG22	1.97	0.46
1:A:795:GLU:C	1:A:798:PRO:HD2	2.36	0.46
2:B:142:PHE:HA	2:B:149:LYS:CG	2.45	0.46
1:A:214:ILE:HG22	1:A:238:PRO:HG3	1.97	0.46
1:A:368:LYS:HD2	1:A:755:ALA:O	2.15	0.46
1:A:567:LEU:HD22	1:A:592:LEU:HD12	1.95	0.46
1:A:797:THR:OG1	1:A:798:PRO:HD3	2.16	0.46
1:A:328:ARG:HA	1:A:331:VAL:CG1	2.45	0.46
1:A:237:SER:HB2	1:A:239:GLU:OE1	2.16	0.46
1:A:855:ASN:OD1	1:A:855:ASN:N	2.47	0.46
1:A:647:SER:HB3	1:A:670:ARG:HD3	1.96	0.46
1:A:801:ILE:HD13	1:A:801:ILE:HA	1.81	0.46
1:A:915:TRP:HD1	2:B:77:LEU:CD2	2.22	0.46
1:A:634:LYS:NZ	1:A:649:THR:HG22	2.31	0.46
1:A:715:GLN:HG3	1:A:721:VAL:HG11	1.96	0.46
1:A:821:LEU:C	1:A:825:ILE:HD11	2.36	0.46
1:A:997:TRP:HA	1:A:1000:VAL:HG23	1.98	0.46
1:A:998:TRP:O	1:A:1001:PRO:HD2	2.16	0.45
1:A:1009:PHE:CD1	1:A:1009:PHE:C	2.90	0.45
1:A:1030:GLU:HB3	1:A:1031:LEU:HD12	1.98	0.45
1:A:823:THR:HG21	1:A:936:GLU:OE2	2.16	0.45
1:A:952:SER:HB2	1:A:1020:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:VAL:HG12	1:A:807:VAL:HG13	1.98	0.45
1:A:388:GLY:HA3	1:A:726:ASP:OD2	2.16	0.45
1:A:389:THR:HG22	1:A:726:ASP:HB3	1.97	0.45
1:A:914:GLU:O	2:B:184:ASN:HB3	2.15	0.45
2:B:74:GLN:HB2	2:B:77:LEU:HD12	1.97	0.45
1:A:279:ILE:HD13	1:A:728:VAL:HG23	1.99	0.45
1:A:776:LEU:HD23	1:A:776:LEU:HA	1.73	0.45
1:A:354:SER:HA	1:A:370:LEU:HD21	1.99	0.45
1:A:396:THR:CG2	1:A:411:THR:HG22	2.47	0.45
1:A:881:ALA:HB2	1:A:930:VAL:HG11	1.99	0.45
1:A:1012:ASP:O	1:A:1016:LYS:HG2	2.15	0.45
1:A:385:BFD:HA	1:A:625:VAL:O	2.16	0.45
1:A:911:TYR:HE2	2:B:70:THR:C	2.20	0.45
1:A:782:LYS:HE3	1:A:853:LEU:O	2.17	0.45
1:A:887:TRP:CE2	1:A:915:TRP:CZ3	3.04	0.45
1:A:931:PHE:O	1:A:935:ILE:HG12	2.17	0.45
1:A:66:THR:HB	1:A:72:LEU:HD13	1.99	0.44
1:A:525:GLU:OE2	1:A:526:ARG:NH1	2.50	0.44
2:B:71:PRO:HG3	2:B:74:GLN:OE1	2.16	0.44
2:B:278:TYR:CD1	2:B:278:TYR:N	2.84	0.44
1:A:227:LEU:HD11	1:A:276:ILE:HG12	1.99	0.44
1:A:339:ALA:HB3	1:A:796:LEU:HD13	1.98	0.44
1:A:557:LEU:HB2	1:A:559:GLU:HG3	1.99	0.44
1:A:208:VAL:HG11	1:A:252:ALA:HB1	1.99	0.44
1:A:605:ARG:HB2	1:A:608:VAL:CG2	2.47	0.44
1:A:952:SER:HB2	1:A:1020:ARG:HH21	1.83	0.44
1:A:49:GLU:HB2	1:A:269:ASN:ND2	2.33	0.44
2:B:213:LEU:HD23	2:B:213:LEU:O	2.17	0.44
1:A:300:PHE:CB	1:A:854:VAL:HG21	2.47	0.44
1:A:883:ALA:HA	1:A:887:TRP:O	2.18	0.44
2:B:188:LYS:HA	2:B:230:PRO:CB	2.47	0.44
1:A:241:THR:HB	1:A:249:ARG:H	1.82	0.44
1:A:112:LEU:HD21	1:A:341:VAL:HG22	2.00	0.44
1:A:784:SER:HA	1:A:831:LEU:CD1	2.48	0.44
2:B:161:ASN:OD1	2:B:161:ASN:N	2.51	0.44
1:A:909:ASP:CB	1:A:915:TRP:CH2	2.93	0.44
1:A:955:GLN:HE22	1:A:1020:ARG:NH1	2.16	0.44
1:A:991:MET:HE3	1:A:991:MET:HB2	1.67	0.44
2:B:159:LEU:HD21	2:B:244:LEU:CD1	2.48	0.44
1:A:96:PRO:HD2	1:A:99:VAL:HG21	2.00	0.43
1:A:441:ALA:HB1	1:A:477:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:HD2	1:A:758:ILE:HD13	2.00	0.43
1:A:273:ARG:HD2	1:A:273:ARG:N	2.33	0.43
1:A:1009:PHE:C	1:A:1009:PHE:HD1	2.21	0.43
2:B:108:GLY:HA2	2:B:111:HIS:HB3	1.99	0.43
2:B:109:LEU:HA	2:B:109:LEU:HD23	1.71	0.43
1:A:291:THR:O	1:A:295:ILE:HG13	2.18	0.43
2:B:213:LEU:HA	2:B:251:ASN:ND2	2.32	0.43
1:A:300:PHE:CD1	1:A:854:VAL:HG11	2.53	0.43
1:A:715:GLN:HG3	1:A:721:VAL:CG1	2.48	0.43
1:A:1019:VAL:HB	1:A:1027:TRP:CD1	2.52	0.43
1:A:64:TYR:CD2	1:A:196:VAL:HG12	2.53	0.43
1:A:66:THR:OG1	1:A:67:SER:N	2.52	0.43
1:A:525:GLU:HG3	1:A:526:ARG:HG3	2.00	0.43
1:A:1011:TYR:OH	2:B:43:TYR:OH	2.08	0.43
2:B:46:ALA:O	2:B:50:VAL:HG23	2.17	0.43
2:B:263:LYS:HA	2:B:281:LYS:HA	2.01	0.43
1:A:95:THR:HB	1:A:100:LYS:HE3	1.99	0.43
1:A:532:ILE:HG22	1:A:533:LYS:HD2	2.00	0.43
1:A:648:GLU:HB3	1:A:652:ASP:HB2	2.00	0.43
1:A:887:TRP:CZ2	1:A:915:TRP:CE3	3.07	0.43
2:B:202:ALA:HA	2:B:213:LEU:HD21	1.99	0.43
1:A:221:LYS:HA	1:A:234:GLN:O	2.19	0.43
1:A:385:BFD:F2	1:A:387:THR:N	2.41	0.43
1:A:687:LEU:HG	1:A:691:LEU:HD12	2.00	0.43
1:A:699:PHE:HB3	1:A:702:THR:HG21	2.01	0.43
1:A:801:ILE:HG21	1:A:875:PHE:CE2	2.53	0.43
1:A:884:GLN:OE1	2:B:73:TYR:HE2	2.02	0.42
2:B:82:VAL:HG11	2:B:264:ILE:HG12	2.01	0.42
2:B:129:ILE:C	2:B:153:LYS:HG3	2.39	0.42
2:B:145:PRO:O	2:B:148:THR:HG22	2.19	0.42
1:A:785:ILE:HD12	1:A:853:LEU:HD22	2.02	0.42
1:A:837:GLU:OE2	1:A:948:THR:HA	2.19	0.42
2:B:180:ILE:CG2	2:B:244:LEU:HD22	2.48	0.42
1:A:51:ASN:OD1	1:A:54:GLN:NE2	2.51	0.42
1:A:203:LYS:O	1:A:258:CYS:HB3	2.18	0.42
1:A:403:ASP:OD2	1:A:424:SER:OG	2.26	0.42
1:A:987:ILE:HG22	1:A:988:PHE:CE1	2.55	0.42
2:B:139:GLN:HB2	2:B:149:LYS:HD2	2.01	0.42
2:B:252:VAL:HA	2:B:253:PRO:HD3	1.94	0.42
1:A:423:SER:O	1:A:428:ARG:NH2	2.46	0.42
1:A:614:LYS:HB3	1:A:768:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TRP:O	2:B:40:ILE:HG22	2.19	0.42
1:A:950:ARG:HG2	1:A:1020:ARG:HB3	2.01	0.42
1:A:524:LEU:HD11	1:A:539:LEU:HD11	2.02	0.42
2:B:224:TYR:CE2	2:B:244:LEU:HA	2.54	0.42
2:B:230:PRO:HD2	2:B:232:TYR:HE1	1.85	0.42
1:A:345:LEU:HA	1:A:348:THR:OG1	2.19	0.42
1:A:352:CYS:SG	1:A:832:ALA:HB2	2.59	0.42
1:A:389:THR:OG1	1:A:390:LEU:N	2.52	0.42
1:A:609:PRO:O	1:A:613:LEU:HG	2.20	0.42
2:B:134:GLU:O	2:B:134:GLU:HG3	2.20	0.42
1:A:112:LEU:CD2	1:A:341:VAL:HG22	2.50	0.42
1:A:300:PHE:HB2	1:A:854:VAL:HG21	2.02	0.42
1:A:830:SER:CB	1:A:964:LEU:HA	2.50	0.41
1:A:840:ILE:HA	1:A:843:LEU:HD12	2.03	0.41
1:A:55:LEU:HD13	1:A:60:LEU:HD23	2.02	0.41
1:A:916:THR:HG22	1:A:919:GLN:CG	2.50	0.41
2:B:203:PHE:HA	2:B:259:VAL:O	2.20	0.41
1:A:110:GLN:O	1:A:114:TRP:CD1	2.73	0.41
1:A:134:THR:C	1:A:136:ASP:H	2.23	0.41
1:A:414:ASP:N	1:A:414:ASP:OD1	2.53	0.41
1:A:440:ALA:HB1	1:A:457:ILE:O	2.20	0.41
1:A:817:LEU:HA	1:A:817:LEU:HD23	1.73	0.41
1:A:939:GLN:OE1	1:A:939:GLN:HA	2.20	0.41
1:A:945:ILE:HG13	1:A:945:ILE:H	1.52	0.41
2:B:74:GLN:HG3	2:B:74:GLN:O	2.21	0.41
2:B:278:TYR:N	2:B:278:TYR:HD1	2.17	0.41
1:A:95:THR:HB	1:A:100:LYS:CE	2.49	0.41
1:A:106:ALA:C	1:A:110:GLN:HG3	2.41	0.41
1:A:124:PHE:CE1	1:A:135:THR:HB	2.56	0.41
1:A:379:THR:HA	1:A:720:ILE:HB	2.02	0.41
1:A:385:BFD:OD1	1:A:707:LYS:NZ	2.53	0.41
1:A:605:ARG:HB2	1:A:608:VAL:HG23	2.02	0.41
1:A:939:GLN:O	1:A:943:VAL:HG12	2.20	0.41
1:A:940:ILE:HD11	1:A:972:VAL:HG13	2.03	0.41
2:B:148:THR:OG1	2:B:149:LYS:N	2.53	0.41
1:A:833:TYR:CB	1:A:961:ASN:HD22	2.34	0.41
1:A:896:ARG:O	1:A:899:TRP:N	2.54	0.41
1:A:909:ASP:CB	1:A:915:TRP:HH2	2.14	0.41
2:B:98:TYR:CD2	2:B:106:TRP:HB3	2.55	0.41
2:B:254:ARG:HA	2:B:254:ARG:HD3	1.88	0.41
1:A:580:PHE:HA	1:A:586:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:TYR:HB2	1:A:961:ASN:HD22	1.86	0.41
1:A:180:VAL:HG22	1:A:181:ILE:N	2.36	0.41
1:A:208:VAL:O	1:A:254:PHE:O	2.39	0.41
1:A:316:PHE:HB2	1:A:333:PHE:HB2	2.01	0.41
1:A:631:ILE:HD12	1:A:631:ILE:H	1.85	0.41
2:B:76:GLN:O	2:B:77:LEU:HD23	2.19	0.41
1:A:798:PRO:CB	1:A:810:PRO:HG2	2.45	0.41
1:A:364:ASN:HB3	1:A:760:LEU:HB2	2.03	0.41
1:A:449:VAL:HG22	1:A:450:PRO:HD2	2.03	0.41
1:A:854:VAL:HG12	1:A:858:LEU:HD23	2.03	0.41
1:A:1025:SER:O	1:A:1029:GLN:HG3	2.20	0.41
2:B:143:LEU:O	2:B:144:ALA:HB2	2.21	0.41
1:A:109:LEU:CB	1:A:346:LEU:HD13	2.45	0.41
1:A:317:ILE:HD13	1:A:317:ILE:HA	1.91	0.40
1:A:581:ASP:N	1:A:586:ASN:HD21	2.17	0.40
1:A:830:SER:HB2	1:A:964:LEU:HA	2.04	0.40
2:B:214:GLN:H	2:B:251:ASN:CG	2.24	0.40
1:A:199:LEU:HD12	1:A:265:GLY:O	2.21	0.40
1:A:809:LEU:HD12	1:A:810:PRO:HD2	2.04	0.40
2:B:224:TYR:HE2	2:B:244:LEU:HA	1.86	0.40
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.73	0.40
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.61	0.40
1:A:310:LEU:O	1:A:314:THR:HG23	2.22	0.40
1:A:786:ALA:CB	1:A:858:LEU:HD11	2.47	0.40
1:A:993:ILE:HG22	1:A:997:TRP:HE3	1.86	0.40
1:A:236:ARG:NH2	1:A:249:ARG:HA	2.35	0.40
1:A:322:ILE:HD12	1:A:322:ILE:HA	1.88	0.40
1:A:489:ILE:O	1:A:498:GLN:HA	2.21	0.40
1:A:809:LEU:HB3	1:A:924:GLN:OE1	2.22	0.40
1:A:866:ILE:O	1:A:870:GLN:HG3	2.21	0.40
1:A:929:THR:HG22	1:A:993:ILE:CD1	2.49	0.40
1:A:64:TYR:CE2	1:A:196:VAL:CG1	3.04	0.40
1:A:134:THR:O	1:A:134:THR:HG22	2.22	0.40
1:A:315:PHE:HA	1:A:318:VAL:HB	2.03	0.40
1:A:1012:ASP:OD1	1:A:1015:ARG:NE	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	984/987 (100%)	933 (95%)	51 (5%)	0	100	100
2	B	252/255 (99%)	231 (92%)	21 (8%)	0	100	100
All	All	1236/1242 (100%)	1164 (94%)	72 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	833/833 (100%)	820 (98%)	13 (2%)	62	81
2	B	222/223 (100%)	216 (97%)	6 (3%)	44	70
All	All	1055/1056 (100%)	1036 (98%)	19 (2%)	59	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	A	272	ASP
1	A	273	ARG
1	A	363	LYS
1	A	438	ASN
1	A	560	ARG
1	A	573	ASP
1	A	756	ASP

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	780	ASN
1	A	826	PHE
1	A	846	ARG
1	A	945	ILE
1	A	1009	PHE
2	B	131	CYS
2	B	158	MET
2	B	165	ARG
2	B	198	ARG
2	B	213	LEU
2	B	257	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	438	ASN
1	A	694	HIS
1	A	913	GLN
1	A	996	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	BFD	A	385	1,3	8,11,12	5.54	3 (37%)	3,15,17	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BFD	A	385	1,3	-	2/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	BFD	F1-BE	9.87	1.78	1.54
1	A	385	BFD	F3-BE	8.99	1.76	1.54
1	A	385	BFD	F2-BE	7.96	1.73	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	385	BFD	CA-CB-CG-OD1
1	A	385	BFD	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	385	BFD	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	B	302	2	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
6	NAG	B	301	2	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
5	J3C	A	1105	-	20,26,26	1.55	4 (20%)	23,39,39	1.84	7 (30%)

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
6	NAG	B	302	2	-	2/6/23/26	0/1/1/1
6	NAG	B	301	2	-	2/6/23/26	0/1/1/1
5	J3C	A	1105	-	-	4/4/20/20	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1105	J3C	C1-N1	-3.82	1.33	1.38
5	A	1105	J3C	C4-N3	-2.74	1.35	1.39
5	A	1105	J3C	C11-C12	2.28	1.55	1.52
5	A	1105	J3C	C5-N2	2.22	1.35	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1105	J3C	C13-C12-N3	-3.68	105.12	110.93
5	A	1105	J3C	C7-N2-C5	3.31	109.43	103.59
5	A	1105	J3C	C10-C8-C7	-3.19	123.85	129.31
6	B	301	NAG	C1-O5-C5	3.01	116.27	112.19
5	A	1105	J3C	C12-C11-C6	2.89	116.81	110.29
5	A	1105	J3C	O2-C11-C12	2.77	114.75	109.01
5	A	1105	J3C	C18-C13-C12	2.50	124.75	120.78
5	A	1105	J3C	C10-C8-N1	2.35	127.90	124.41
6	B	302	NAG	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

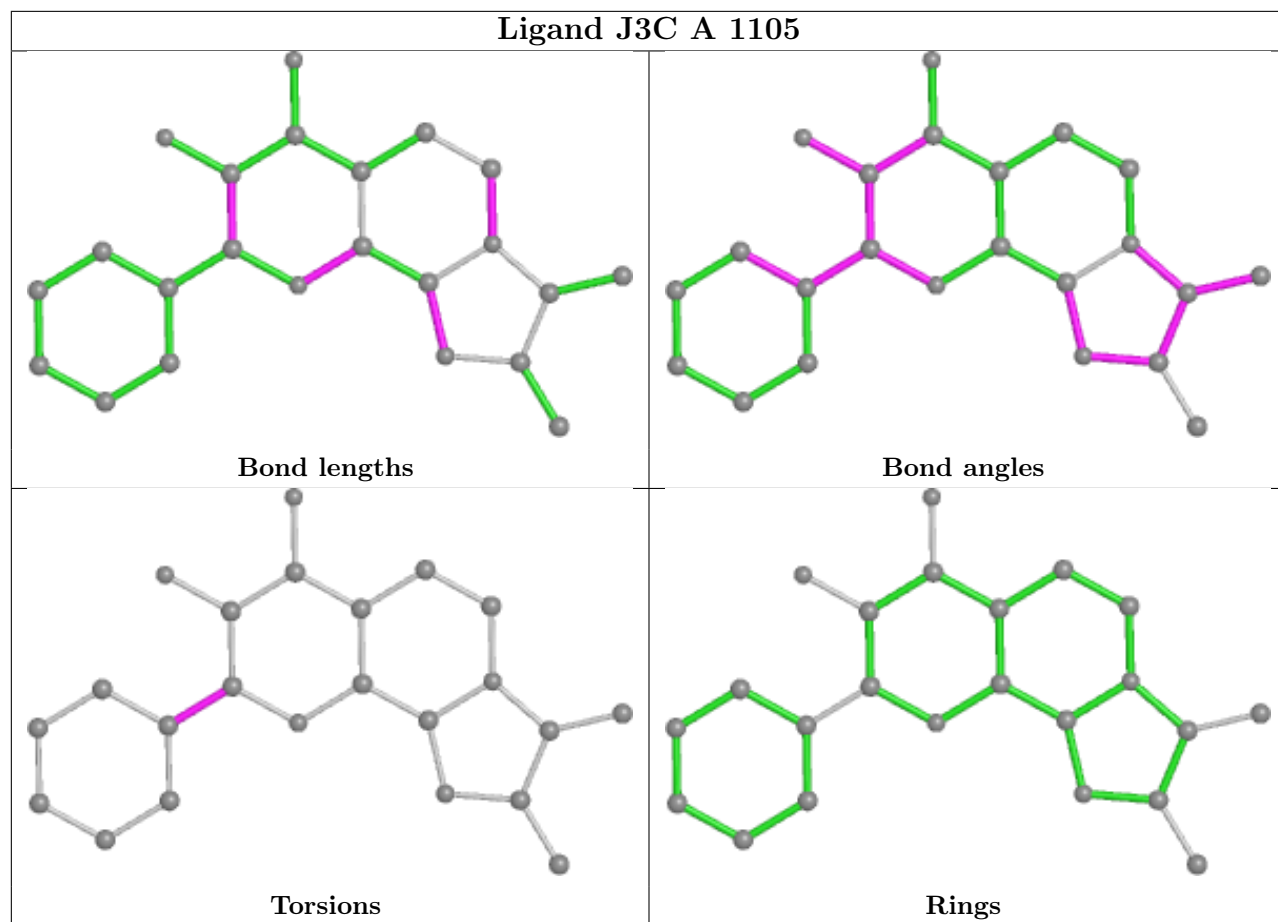


Mol	Chain	Res	Type	Atoms
6	B	302	NAG	O5-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
6	B	302	NAG	C4-C5-C6-O6
6	B	301	NAG	C4-C5-C6-O6
5	A	1105	J3C	N3-C12-C13-C14
5	A	1105	J3C	N3-C12-C13-C18
5	A	1105	J3C	C11-C12-C13-C14
5	A	1105	J3C	C11-C12-C13-C18

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	986/987 (99%)	-0.25	14 (1%) 75 74	59, 92, 143, 197	0
2	B	254/255 (99%)	-0.05	2 (0%) 86 85	78, 120, 157, 191	0
All	All	1240/1242 (99%)	-0.21	16 (1%) 77 76	59, 98, 151, 197	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	5.2
1	A	173	LEU	4.4
2	B	39	TRP	4.0
1	A	48	MET	3.8
1	A	49	GLU	3.7
1	A	958	PHE	3.5
2	B	229	PHE	3.1
1	A	494	THR	2.8
1	A	487	CYS	2.6
1	A	50	ILE	2.5
1	A	501	ILE	2.5
1	A	512	HIS	2.5
1	A	1025	SER	2.4
1	A	959	PHE	2.4
1	A	436	LEU	2.2
1	A	438	ASN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	BFD	A	385	12/13	0.90	0.23	71,74,77,87	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

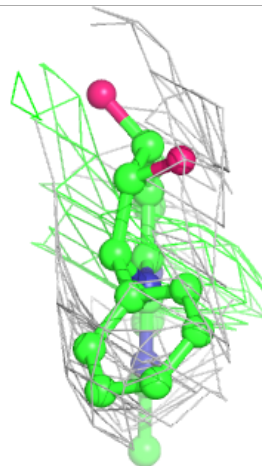
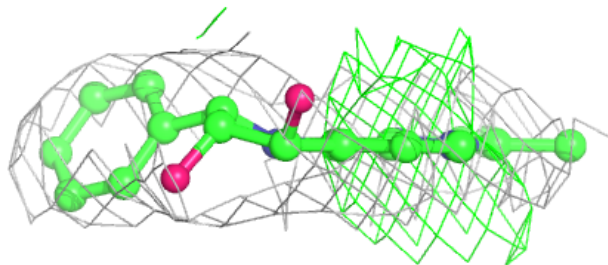
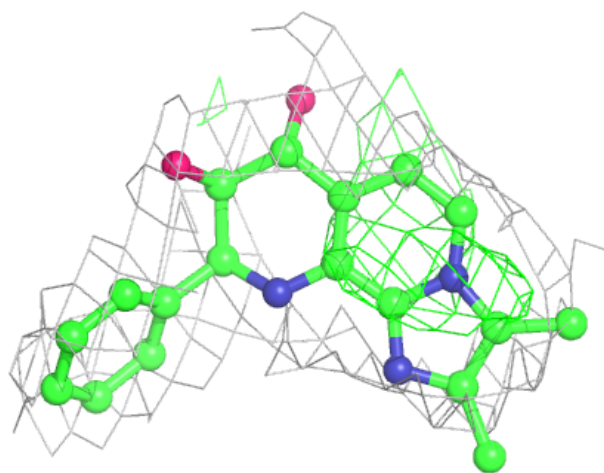
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	302	14/15	0.83	0.28	115,127,136,141	0
6	NAG	B	301	14/15	0.91	0.25	82,85,99,100	0
3	MG	A	1101	1/1	0.91	0.29	70,70,70,70	0
4	RB	A	1104	1/1	0.92	0.32	156,156,156,156	0
5	J3C	A	1105	23/23	0.93	0.27	83,86,91,91	0
4	RB	B	303	1/1	0.97	0.29	190,190,190,190	0
4	RB	A	1103	1/1	0.98	0.16	113,113,113,113	0
4	RB	A	1102	1/1	0.98	0.17	137,137,137,137	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.

**Electron density around J3C A 1105:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.