



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:48 AM UTC

PDB ID : 7EFM / pdb_00007efm
Title : Crystal structure of the gastric proton pump K791S/E820D/Y340N in (BYK)E2BeF state
Authors : Abe, K.; Yamamoto, K.; Irie, K.
Deposited on : 2021-03-22
Resolution : 3.20 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

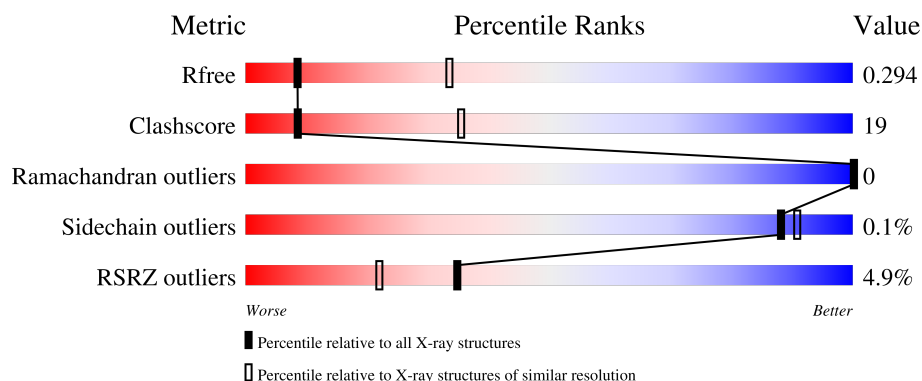
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	4% 66% 34%
2	B	261	8% 63% 37%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9816 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
			7655	1	4881	3	1292	1424	54			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP A0A5G2QYH2
A	340	ASN	TYR	engineered mutation	UNP A0A5G2QYH2
A	791	SER	LYS	engineered mutation	UNP A0A5G2QYH2
A	820	ASP	GLU	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	261	Total	C	N	O	S	0	0	0
			2092	1359	347	375	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

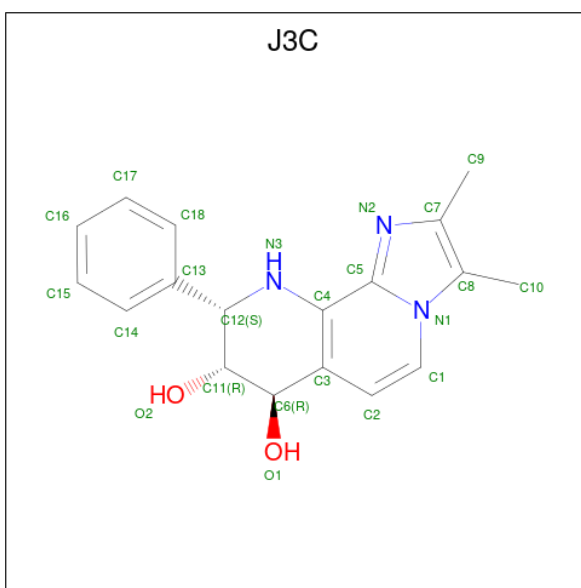
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

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

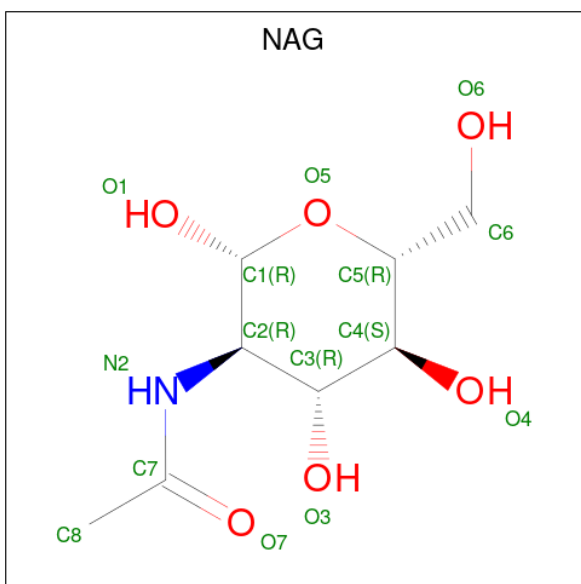
- Molecule 5 is (7R,8R,9S)-2,3-dimethyl-9-phenyl-7,8,9,10-tetrahydroimidazo[1,2-h][1,7]naphthyridine-7,8-diol (CCD ID: J3C) (formula: C₁₈H₁₉N₃O₂) (labeled as "Ligand of Interest")

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 (CCD ID: 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		

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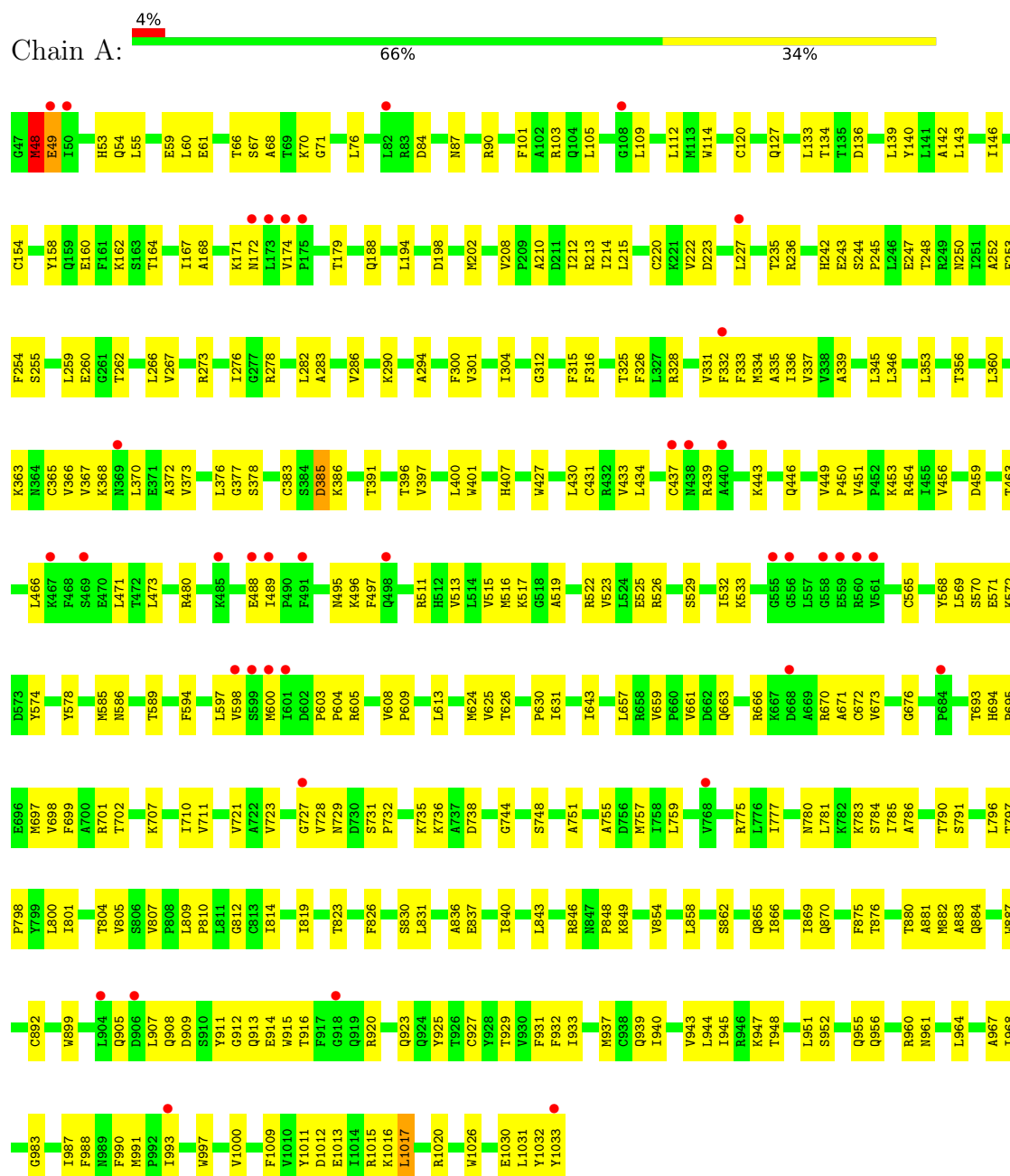
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

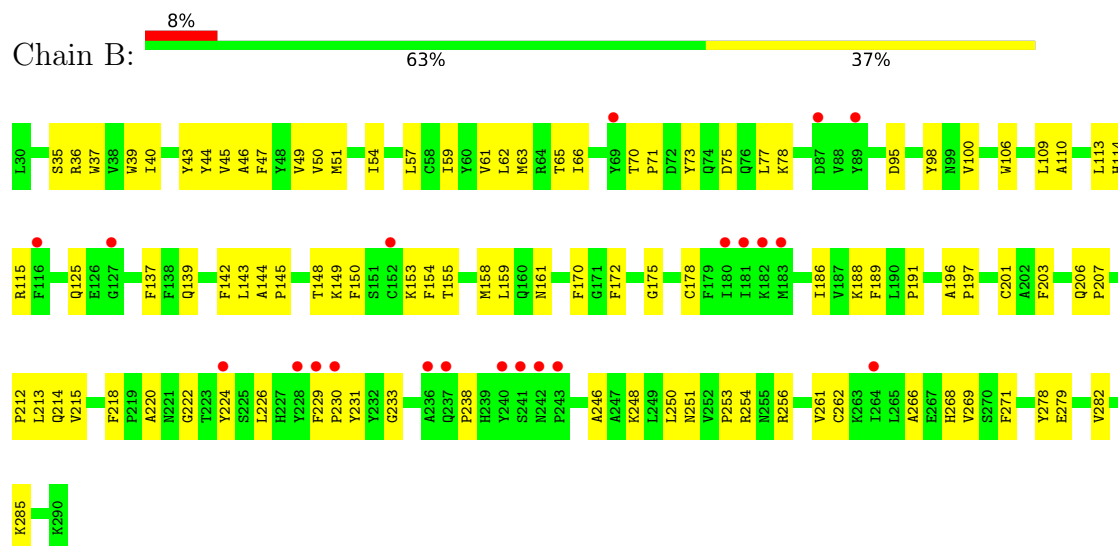
3 Residue-property plots

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, α , β , γ	104.69Å 104.69Å 368.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.15 – 3.20 48.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.15-3.20) 94.8 (48.15-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.228 , 0.293 (Not available) , 0.294	Depositor DCC
R_{free} test set	1958 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9816	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/7799	0.76	5/10593 (0.0%)
2	B	0.40	0/2159	0.67	0/2937
All	All	0.46	0/9958	0.74	5/13530 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	MET	N-CA-C	8.32	121.33	110.43
1	A	49	GLU	N-CA-C	7.90	119.53	111.07
1	A	1017	LEU	N-CA-C	-5.35	105.89	112.90
1	A	812	GLY	CA-C-N	-5.06	114.25	122.65
1	A	812	GLY	C-N-CA	-5.06	114.25	122.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7655	0	7672	291	0
2	B	2092	0	2039	91	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	23	0	0	0	0
6	B	42	0	39	1	0
All	All	9816	0	9750	369	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 19.

All (369) 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:400:LEU:HD21	1:A:598:VAL:CG2	1.44	1.47
1:A:400:LEU:CD2	1:A:598:VAL:HG22	1.50	1.40
1:A:400:LEU:HD23	1:A:597:LEU:O	1.50	1.10
1:A:48:MET:HA	1:A:48:MET:HE3	1.40	1.03
1:A:905:GLN:HG3	2:B:278:TYR:CE2	1.96	0.99
1:A:227:LEU:HD21	1:A:276:ILE:HG12	1.39	0.98
1:A:400:LEU:HD23	1:A:598:VAL:HA	1.46	0.98
1:A:400:LEU:CD2	1:A:597:LEU:O	2.15	0.95
1:A:312:GLY:HA2	1:A:336:ILE:HD11	1.50	0.92
1:A:798:PRO:HB3	1:A:810:PRO:HG2	1.52	0.91
1:A:1015:ARG:HH11	1:A:1032:TYR:HA	1.37	0.90
2:B:214:GLN:H	2:B:251:ASN:HB2	1.39	0.88
1:A:945:ILE:HD11	1:A:1009:PHE:HA	1.60	0.83
1:A:905:GLN:O	1:A:916:THR:HA	1.78	0.83
1:A:804:THR:HG23	1:A:805:VAL:HG13	1.60	0.82
1:A:1017:LEU:HD13	1:A:1020:ARG:HH12	1.41	0.82
1:A:227:LEU:HD21	1:A:276:ILE:CG1	2.11	0.80
1:A:400:LEU:CD2	1:A:598:VAL:HA	2.12	0.79
1:A:727:GLY:O	1:A:751:ALA:HB2	1.83	0.78
1:A:929:THR:HB	1:A:993:ILE:HD11	1.67	0.77
1:A:49:GLU:HG2	1:A:245:PRO:HG2	1.65	0.76
1:A:1017:LEU:CD1	1:A:1020:ARG:NH1	2.49	0.76
2:B:114:HIS:HB3	2:B:115:ARG:HH11	1.49	0.76
1:A:400:LEU:HD23	1:A:598:VAL:CA	2.15	0.76
1:A:699:PHE:HB3	1:A:702:THR:HG21	1.68	0.76
2:B:206:GLN:OE1	2:B:256:ARG:NH2	2.19	0.76
1:A:53:HIS:HE1	1:A:245:PRO:HG3	1.49	0.75
1:A:55:LEU:HD22	1:A:59:GLU:HB3	1.68	0.75
1:A:1017:LEU:HD13	1:A:1020:ARG:NH1	2.00	0.75
1:A:925:TYR:C	1:A:991:MET:HE1	2.12	0.74
1:A:1015:ARG:NH1	1:A:1032:TYR:HA	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ILE:HA	2:B:62:LEU:HB3	1.67	0.74
1:A:805:VAL:HG23	1:A:807:VAL:HG13	1.70	0.74
1:A:210:ALA:HA	1:A:254:PHE:HD1	1.54	0.73
1:A:400:LEU:HD21	1:A:598:VAL:CB	2.17	0.72
1:A:1012:ASP:HA	1:A:1015:ARG:HG2	1.71	0.72
1:A:400:LEU:CD2	1:A:598:VAL:CG2	2.34	0.72
1:A:905:GLN:HG3	2:B:278:TYR:HE2	1.52	0.71
1:A:801:ILE:HA	1:A:804:THR:HG22	1.73	0.70
2:B:159:LEU:HD23	2:B:246:ALA:HB2	1.73	0.70
1:A:133:LEU:O	1:A:134:THR:HG22	1.91	0.70
2:B:155:THR:H	2:B:158:MET:HE1	1.57	0.70
1:A:887:TRP:HH2	1:A:915:TRP:CD2	2.09	0.69
1:A:48:MET:HA	1:A:48:MET:CE	2.22	0.69
2:B:196:ALA:HA	2:B:226:LEU:HD11	1.75	0.68
2:B:212:PRO:O	2:B:251:ASN:ND2	2.27	0.68
1:A:168:ALA:HA	1:A:171:LYS:HD3	1.74	0.68
1:A:433:VAL:HG23	1:A:515:VAL:HB	1.75	0.67
1:A:439:ARG:NH2	1:A:488:GLU:OE2	2.26	0.67
1:A:53:HIS:CE1	1:A:245:PRO:HG3	2.28	0.67
1:A:624:MET:HE2	1:A:698:VAL:HG13	1.77	0.67
2:B:62:LEU:O	2:B:66:ILE:HG13	1.94	0.67
1:A:790:THR:HG22	1:A:862:SER:HB3	1.77	0.67
1:A:356:THR:HB	1:A:373:VAL:HG11	1.77	0.66
1:A:784:SER:HA	1:A:831:LEU:HD12	1.78	0.66
2:B:250:LEU:HD21	6:B:303:NAG:H81	1.78	0.66
1:A:882:MET:CE	1:A:923:GLN:HE21	2.09	0.66
1:A:948:THR:HG21	1:A:956:GLN:HG3	1.76	0.66
1:A:1012:ASP:OD1	1:A:1015:ARG:NH2	2.28	0.66
1:A:227:LEU:O	1:A:729:ASN:HB3	1.96	0.65
1:A:943:VAL:HG22	1:A:964:LEU:HD11	1.80	0.64
1:A:1011:TYR:HH	2:B:43:TYR:HH	1.44	0.64
2:B:46:ALA:O	2:B:50:VAL:HG23	1.97	0.63
1:A:210:ALA:O	1:A:254:PHE:HA	1.99	0.63
1:A:400:LEU:CD2	1:A:598:VAL:CA	2.75	0.63
1:A:905:GLN:CG	2:B:278:TYR:CE2	2.67	0.63
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.81	0.63
1:A:356:THR:OG1	1:A:777:ILE:HG21	1.99	0.62
1:A:400:LEU:HD23	1:A:597:LEU:C	2.23	0.62
1:A:312:GLY:HA2	1:A:336:ILE:CD1	2.27	0.62
1:A:882:MET:HE2	1:A:923:GLN:HE21	1.65	0.62
1:A:908:GLN:HA	1:A:913:GLN:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:SER:OG	1:A:964:LEU:HA	1.99	0.62
2:B:148:THR:HG23	2:B:238:PRO:HD2	1.82	0.62
2:B:203:PHE:CD2	2:B:206:GLN:HB2	2.35	0.62
1:A:809:LEU:HD12	1:A:810:PRO:HD2	1.82	0.61
1:A:386:LYS:HB2	1:A:626:THR:HG21	1.82	0.61
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.35	0.61
1:A:49:GLU:CG	1:A:245:PRO:HG2	2.31	0.61
1:A:325:THR:H	1:A:328:ARG:HH21	1.49	0.60
1:A:837:GLU:HB3	1:A:951:LEU:HD13	1.82	0.60
1:A:360:LEU:O	1:A:363:LYS:N	2.29	0.60
1:A:386:LYS:HB2	1:A:626:THR:CG2	2.32	0.60
1:A:783:LYS:NZ	1:A:837:GLU:OE1	2.32	0.59
2:B:59:ILE:O	2:B:63:MET:N	2.25	0.59
1:A:585:MET:HE2	1:A:589:THR:CG2	2.32	0.59
1:A:513:VAL:HG22	1:A:568:TYR:CE1	2.38	0.59
1:A:431:CYS:SG	1:A:473:LEU:HD12	2.41	0.59
1:A:676:GLY:H	1:A:701:ARG:HB2	1.68	0.58
1:A:76:LEU:HD12	1:A:76:LEU:O	2.04	0.58
1:A:227:LEU:HD11	1:A:253:PHE:HB3	1.86	0.58
2:B:203:PHE:HZ	2:B:253:PRO:HD3	1.68	0.58
1:A:1017:LEU:HD12	1:A:1020:ARG:NH1	2.18	0.58
1:A:911:TYR:CE2	2:B:71:PRO:HA	2.39	0.57
1:A:876:THR:O	1:A:880:THR:HG23	2.05	0.57
1:A:1011:TYR:OH	2:B:43:TYR:OH	2.17	0.57
1:A:109:LEU:HB2	1:A:346:LEU:HD12	1.86	0.57
2:B:98:TYR:CD2	2:B:106:TRP:HB3	2.40	0.57
1:A:880:THR:HG22	2:B:62:LEU:HD22	1.86	0.57
1:A:139:LEU:O	1:A:143:LEU:CD2	2.53	0.57
1:A:609:PRO:O	1:A:613:LEU:HG	2.05	0.57
1:A:449:VAL:HG23	1:A:454:ARG:HG2	1.86	0.56
1:A:605:ARG:HB2	1:A:608:VAL:CG2	2.34	0.56
1:A:242:HIS:CE1	1:A:244:SER:HB3	2.41	0.56
1:A:120:CYS:CB	1:A:142:ALA:HB2	2.35	0.56
1:A:255:SER:HB3	1:A:276:ILE:HD13	1.87	0.56
1:A:353:LEU:HB2	1:A:370:LEU:HD13	1.88	0.56
1:A:947:LYS:HZ1	1:A:961:ASN:H	1.51	0.56
2:B:145:PRO:O	2:B:148:THR:OG1	2.18	0.56
1:A:53:HIS:HB2	1:A:250:ASN:HD21	1.71	0.56
1:A:672:CYS:HB2	1:A:694:HIS:ND1	2.20	0.55
1:A:61:GLU:HB2	1:A:66:THR:O	2.05	0.55
1:A:300:PHE:CZ	1:A:304:ILE:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TRP:HB3	1:A:597:LEU:HB2	1.89	0.55
1:A:661:VAL:O	1:A:666:ARG:NH2	2.39	0.55
1:A:659:VAL:HG12	1:A:663:GLN:HB2	1.88	0.55
1:A:53:HIS:HA	1:A:213:ARG:HD3	1.86	0.55
1:A:881:ALA:HA	1:A:997:TRP:CZ2	2.40	0.55
1:A:585:MET:HE2	1:A:589:THR:HG21	1.89	0.55
1:A:630:PRO:HB3	1:A:673:VAL:HG11	1.88	0.55
1:A:139:LEU:O	1:A:143:LEU:HD23	2.06	0.54
2:B:37:TRP:CE3	2:B:40:ILE:HD11	2.41	0.54
1:A:242:HIS:ND1	1:A:247:GLU:HB2	2.23	0.54
1:A:777:ILE:HA	1:A:780:ASN:HB2	1.90	0.54
1:A:120:CYS:HB3	1:A:142:ALA:HB2	1.90	0.54
2:B:125:GLN:O	2:B:153:LYS:NZ	2.40	0.54
1:A:731:SER:OG	1:A:732:PRO:HD3	2.08	0.54
1:A:179:THR:HG22	1:A:188:GLN:HG2	1.90	0.53
1:A:87:ASN:HD22	1:A:194:LEU:HB2	1.73	0.53
1:A:569:LEU:HB3	1:A:574:TYR:CD2	2.43	0.53
1:A:1026:TRP:CZ3	1:A:1030:GLU:HG3	2.44	0.53
1:A:227:LEU:CD2	1:A:276:ILE:HG12	2.28	0.53
1:A:345:LEU:HD11	1:A:785:ILE:HG12	1.90	0.53
1:A:1017:LEU:HA	1:A:1020:ARG:CZ	2.38	0.53
1:A:396:THR:OG1	1:A:603:PRO:HG3	2.09	0.53
1:A:459:ASP:O	1:A:463:THR:HG23	2.09	0.52
2:B:36:ARG:NH1	2:B:39:TRP:HB2	2.24	0.52
1:A:114:TRP:HZ3	1:A:146:ILE:HD13	1.74	0.52
1:A:133:LEU:O	1:A:134:THR:CG2	2.57	0.52
1:A:940:ILE:HG23	1:A:968:ILE:HD13	1.92	0.52
1:A:365:CYS:SG	1:A:757:MET:HE2	2.50	0.52
1:A:227:LEU:HD23	1:A:728:VAL:CG2	2.40	0.52
1:A:235:THR:O	1:A:236:ARG:HD2	2.09	0.52
2:B:266:ALA:HB3	2:B:269:VAL:HB	1.90	0.52
1:A:956:GLN:HB3	1:A:960:ARG:HD2	1.91	0.52
1:A:814:ILE:HD11	1:A:988:PHE:HD1	1.75	0.51
1:A:887:TRP:CH2	1:A:915:TRP:CD2	2.97	0.51
1:A:136:ASP:HB3	1:A:140:TYR:CE2	2.45	0.51
1:A:202:MET:HE3	1:A:208:VAL:HG22	1.93	0.51
1:A:854:VAL:HA	1:A:858:LEU:HD23	1.92	0.51
2:B:36:ARG:HH11	2:B:39:TRP:HB2	1.76	0.51
1:A:212:ILE:HB	1:A:252:ALA:HB3	1.93	0.51
1:A:840:ILE:HA	1:A:843:LEU:HD12	1.93	0.51
2:B:57:LEU:O	2:B:61:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ALA:HB1	1:A:840:ILE:HG13	1.92	0.51
2:B:262:CYS:HB2	2:B:282:VAL:HG23	1.93	0.51
1:A:869:ILE:HG12	2:B:51:MET:HE2	1.92	0.50
1:A:158:TYR:CE2	1:A:162:LYS:HD2	2.46	0.50
1:A:882:MET:HE3	1:A:927:CYS:SG	2.51	0.50
1:A:529:SER:O	1:A:594:PHE:N	2.29	0.50
2:B:51:MET:HE1	2:B:54:ILE:HD11	1.94	0.50
2:B:159:LEU:HA	2:B:218:PHE:HB3	1.92	0.50
1:A:101:PHE:HE2	1:A:154:CYS:HG	1.60	0.50
1:A:944:LEU:O	1:A:947:LYS:HB2	2.12	0.50
1:A:676:GLY:HA3	1:A:701:ARG:O	2.12	0.50
1:A:849:LYS:HD2	1:A:849:LYS:N	2.27	0.50
1:A:711:VAL:HG13	1:A:721:VAL:HG11	1.93	0.50
2:B:43:TYR:O	2:B:47:PHE:N	2.39	0.50
1:A:68:ALA:HB1	1:A:215:LEU:HD13	1.93	0.49
1:A:866:ILE:O	1:A:870:GLN:HG3	2.12	0.49
2:B:161:ASN:HB2	2:B:218:PHE:CE2	2.47	0.49
1:A:300:PHE:CD1	1:A:854:VAL:HG21	2.48	0.49
1:A:511:ARG:HB2	1:A:569:LEU:O	2.11	0.49
1:A:451:VAL:HG11	1:A:471:LEU:HG	1.94	0.49
1:A:84:ASP:HB3	1:A:273:ARG:HH12	1.78	0.49
2:B:203:PHE:HD2	2:B:206:GLN:HB2	1.74	0.49
2:B:203:PHE:CD1	2:B:213:LEU:HB2	2.48	0.49
1:A:400:LEU:HD22	1:A:597:LEU:O	2.08	0.49
2:B:142:PHE:HA	2:B:149:LYS:HG2	1.94	0.49
2:B:178:CYS:SG	2:B:248:LYS:HB2	2.52	0.49
1:A:213:ARG:NH1	1:A:214:ILE:O	2.46	0.48
1:A:283:ALA:O	1:A:735:LYS:HD2	2.13	0.48
2:B:35:SER:HB2	2:B:36:ARG:NH2	2.28	0.48
1:A:925:TYR:O	1:A:991:MET:HE1	2.12	0.48
1:A:430:LEU:HA	1:A:433:VAL:HG12	1.95	0.48
1:A:624:MET:HE3	1:A:626:THR:HG23	1.95	0.48
2:B:36:ARG:NH1	2:B:36:ARG:HA	2.28	0.48
1:A:798:PRO:HG3	1:A:931:PHE:CE1	2.49	0.48
2:B:51:MET:CE	2:B:54:ILE:HD11	2.44	0.48
1:A:532:ILE:HG22	1:A:533:LYS:HD2	1.96	0.48
1:A:586:ASN:OD1	1:A:586:ASN:N	2.40	0.48
1:A:325:THR:HG23	1:A:328:ARG:NH2	2.29	0.48
1:A:916:THR:O	1:A:920:ARG:HG2	2.14	0.48
1:A:932:PHE:CD1	1:A:933:ILE:HG13	2.49	0.48
2:B:191:PRO:C	2:B:268:HIS:HB2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:TYR:CE2	2:B:233:GLY:HA2	2.49	0.48
1:A:242:HIS:ND1	1:A:244:SER:HB3	2.29	0.47
1:A:875:PHE:CD1	1:A:931:PHE:HE2	2.32	0.47
1:A:167:ILE:HG13	1:A:366:VAL:HG11	1.96	0.47
1:A:819:ILE:HA	1:A:823:THR:OG1	2.14	0.47
2:B:110:ALA:O	2:B:113:LEU:N	2.47	0.47
2:B:139:GLN:HB3	2:B:149:LYS:HD2	1.95	0.47
2:B:148:THR:HG23	2:B:238:PRO:CD	2.44	0.47
2:B:203:PHE:HD1	2:B:213:LEU:HB2	1.79	0.47
1:A:495:ASN:HB2	1:A:497:PHE:CZ	2.49	0.47
1:A:780:ASN:HA	1:A:783:LYS:HD2	1.96	0.47
1:A:54:GLN:OE1	1:A:243:GLU:HG2	2.14	0.47
1:A:198:ASP:O	1:A:267:VAL:HG23	2.15	0.47
2:B:186:ILE:HB	2:B:189:PHE:HB2	1.96	0.47
1:A:368:LYS:HD2	1:A:755:ALA:O	2.14	0.47
1:A:797:THR:OG1	1:A:798:PRO:HD3	2.14	0.47
1:A:915:TRP:CE2	2:B:77:LEU:HD11	2.49	0.47
2:B:35:SER:HB2	2:B:36:ARG:HH21	1.78	0.47
2:B:95:ASP:HA	2:B:285:LYS:HB2	1.97	0.47
1:A:339:ALA:HB3	1:A:796:LEU:HD13	1.97	0.47
2:B:114:HIS:CE1	2:B:170:PHE:HE1	2.33	0.47
1:A:53:HIS:HB2	1:A:250:ASN:ND2	2.30	0.47
2:B:45:VAL:O	2:B:49:VAL:HG13	2.15	0.46
1:A:223:ASP:HB2	1:A:259:LEU:HD11	1.97	0.46
1:A:525:GLU:HG3	1:A:526:ARG:HG3	1.97	0.46
1:A:397:VAL:HG22	1:A:600:MET:HG2	1.96	0.46
1:A:657:LEU:O	1:A:659:VAL:HG23	2.16	0.46
2:B:61:VAL:O	2:B:65:THR:HG23	2.16	0.46
2:B:201:CYS:HA	2:B:261:VAL:O	2.16	0.46
1:A:1013:GLU:O	1:A:1017:LEU:N	2.48	0.46
1:A:315:PHE:CZ	1:A:800:LEU:HD13	2.51	0.46
1:A:571:GLU:H	1:A:571:GLU:CD	2.23	0.46
2:B:144:ALA:HB3	2:B:148:THR:HB	1.97	0.46
1:A:90:ARG:HA	1:A:90:ARG:HD2	1.67	0.46
1:A:333:PHE:O	1:A:337:VAL:HG13	2.16	0.46
1:A:443:LYS:C	1:A:446:GLN:HE21	2.24	0.46
1:A:516:MET:HB3	1:A:565:CYS:SG	2.55	0.46
2:B:37:TRP:HA	2:B:40:ILE:HG12	1.97	0.46
1:A:220:CYS:HB2	1:A:262:THR:O	2.16	0.46
1:A:1015:ARG:HH22	1:A:1033:TYR:HE1	1.64	0.45
1:A:721:VAL:O	1:A:738:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TYR:OH	1:A:586:ASN:HB2	2.16	0.45
1:A:791:SER:HB3	1:A:939:GLN:NE2	2.31	0.45
1:A:427:TRP:CH2	1:A:431:CYS:HB2	2.52	0.45
2:B:63:MET:HE2	2:B:63:MET:HA	1.97	0.45
1:A:400:LEU:CD2	1:A:598:VAL:CB	2.88	0.45
1:A:519:ALA:O	1:A:523:VAL:HG23	2.17	0.45
1:A:1030:GLU:HB2	1:A:1031:LEU:HD22	1.98	0.45
2:B:175:GLY:HA3	2:B:254:ARG:NH2	2.31	0.45
1:A:884:GLN:HG2	2:B:73:TYR:HD1	1.82	0.45
1:A:907:LEU:O	1:A:914:GLU:HA	2.16	0.45
2:B:137:PHE:CE1	2:B:139:GLN:HB2	2.52	0.45
1:A:385:BFD:HA	1:A:625:VAL:O	2.17	0.45
1:A:456:VAL:CG1	1:A:463:THR:HG22	2.47	0.45
1:A:53:HIS:HA	1:A:213:ARG:CD	2.47	0.45
1:A:172:ASN:OD1	1:A:174:VAL:HG12	2.17	0.45
1:A:496:LYS:HG3	1:A:522:ARG:HE	1.82	0.45
1:A:952:SER:HB2	1:A:1020:ARG:NH2	2.31	0.45
2:B:114:HIS:CE1	2:B:170:PHE:CE1	3.05	0.45
1:A:378:SER:HB3	1:A:846:ARG:NH1	2.31	0.44
1:A:707:LYS:O	1:A:711:VAL:HG23	2.17	0.44
2:B:188:LYS:HA	2:B:230:PRO:CB	2.47	0.44
2:B:214:GLN:H	2:B:251:ASN:CB	2.19	0.44
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.77	0.44
1:A:385:BFD:F1	1:A:729:ASN:ND2	2.40	0.44
2:B:139:GLN:CD	2:B:150:PHE:H	2.26	0.44
1:A:450:PRO:HD2	1:A:453:LYS:HD3	1.98	0.44
1:A:466:LEU:HD13	1:A:480:ARG:HH22	1.82	0.44
1:A:909:ASP:OD1	1:A:912:GLY:N	2.49	0.44
1:A:127:GLN:HE21	1:A:331:VAL:HG11	1.82	0.44
2:B:148:THR:HG22	2:B:149:LYS:N	2.33	0.44
1:A:339:ALA:CB	1:A:796:LEU:HD13	2.48	0.44
1:A:516:MET:HE2	1:A:523:VAL:HG13	2.00	0.44
2:B:73:TYR:HB3	2:B:75:ASP:CG	2.43	0.44
2:B:191:PRO:HG3	2:B:229:PHE:CE2	2.53	0.44
2:B:191:PRO:O	2:B:266:ALA:HB1	2.17	0.44
1:A:826:PHE:CD2	1:A:967:ALA:HA	2.52	0.44
2:B:262:CYS:HB2	2:B:282:VAL:CG2	2.47	0.44
1:A:400:LEU:HD21	1:A:598:VAL:HG22	0.58	0.44
1:A:899:TRP:CZ2	1:A:920:ARG:HB2	2.53	0.44
1:A:427:TRP:CZ2	1:A:431:CYS:HB2	2.53	0.44
1:A:356:THR:O	1:A:360:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HG	2:B:215:VAL:CG2	2.48	0.43
1:A:952:SER:HB3	1:A:955:GLN:HG2	2.00	0.43
1:A:140:TYR:HA	1:A:143:LEU:CD2	2.49	0.43
1:A:160:GLU:O	1:A:164:THR:HG23	2.17	0.43
1:A:446:GLN:HB3	1:A:449:VAL:HG22	2.00	0.43
1:A:570:SER:OG	1:A:572:LYS:HG2	2.18	0.43
2:B:75:ASP:O	2:B:78:LYS:NZ	2.51	0.43
1:A:643:ILE:HG23	1:A:671:ALA:HB2	2.00	0.43
1:A:727:GLY:HA2	1:A:748:SER:HB3	2.01	0.43
1:A:798:PRO:CB	1:A:810:PRO:HG2	2.34	0.43
1:A:846:ARG:O	1:A:848:PRO:HD3	2.18	0.43
1:A:1016:LYS:O	1:A:1020:ARG:HG2	2.18	0.43
1:A:283:ALA:O	1:A:286:VAL:HB	2.19	0.43
1:A:391:THR:HA	1:A:604:PRO:HA	2.01	0.43
1:A:578:TYR:C	1:A:578:TYR:CD2	2.96	0.43
1:A:624:MET:HE3	1:A:626:THR:CG2	2.49	0.43
1:A:139:LEU:O	1:A:143:LEU:HD22	2.18	0.43
1:A:377:GLY:HA2	1:A:775:ARG:HG3	2.00	0.43
1:A:431:CYS:HA	1:A:434:LEU:HG	2.00	0.43
1:A:983:GLY:O	1:A:987:ILE:HG13	2.19	0.43
1:A:473:LEU:HD23	1:A:473:LEU:O	2.19	0.43
1:A:67:SER:CB	1:A:70:LYS:H	2.32	0.43
1:A:334:MET:O	1:A:335:ALA:C	2.61	0.43
1:A:446:GLN:HB3	1:A:449:VAL:CG2	2.48	0.43
1:A:227:LEU:HD12	1:A:253:PHE:CD2	2.53	0.43
1:A:282:LEU:HD22	1:A:732:PRO:HG3	2.00	0.43
1:A:367:VAL:CG1	1:A:372:ALA:HB3	2.48	0.43
1:A:865:GLN:HE21	2:B:44:TYR:HE1	1.67	0.43
1:A:932:PHE:HD1	1:A:933:ILE:HG13	1.82	0.43
1:A:236:ARG:NH2	1:A:248:THR:O	2.52	0.42
1:A:316:PHE:HB2	1:A:333:PHE:HB2	2.00	0.42
1:A:222:VAL:HG12	1:A:223:ASP:N	2.34	0.42
2:B:271:PHE:HA	2:B:279:GLU:O	2.19	0.42
1:A:103:ARG:C	1:A:105:LEU:H	2.27	0.42
1:A:887:TRP:CH2	1:A:915:TRP:CE2	3.07	0.42
2:B:125:GLN:NE2	2:B:154:PHE:O	2.47	0.42
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.90	0.42
1:A:1031:LEU:HD11	2:B:43:TYR:CE2	2.55	0.42
2:B:36:ARG:HA	2:B:36:ARG:CZ	2.50	0.42
1:A:325:THR:O	1:A:326:PHE:C	2.63	0.42
1:A:489:ILE:HG21	1:A:489:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:TRP:HA	1:A:1000:VAL:HG23	2.00	0.42
1:A:112:LEU:HD22	1:A:301:VAL:HG13	2.02	0.42
1:A:937:MET:HE2	1:A:937:MET:HA	2.00	0.42
1:A:670:ARG:O	1:A:695:PRO:HD2	2.20	0.42
1:A:790:THR:HG22	1:A:862:SER:CB	2.48	0.42
1:A:929:THR:OG1	1:A:990:PHE:HA	2.19	0.42
1:A:220:CYS:HA	1:A:260:GLU:O	2.20	0.41
1:A:400:LEU:O	1:A:407:HIS:HD2	2.03	0.41
1:A:759:LEU:HA	1:A:759:LEU:HD23	1.79	0.41
2:B:186:ILE:HB	2:B:189:PHE:CB	2.50	0.41
1:A:49:GLU:HB2	1:A:278:ARG:HH22	1.84	0.41
1:A:332:PHE:O	1:A:336:ILE:HG23	2.20	0.41
1:A:781:LEU:HD23	1:A:781:LEU:HA	1.92	0.41
1:A:882:MET:HE2	1:A:882:MET:HA	2.02	0.41
1:A:212:ILE:HA	1:A:266:LEU:O	2.20	0.41
1:A:290:LYS:HG2	1:A:294:ALA:HB3	2.01	0.41
2:B:46:ALA:O	2:B:49:VAL:HG22	2.20	0.41
2:B:109:LEU:HD13	2:B:172:PHE:CE1	2.55	0.41
1:A:693:THR:HG22	1:A:694:HIS:CD2	2.55	0.41
1:A:988:PHE:HB2	1:A:990:PHE:HD2	1.85	0.41
1:A:255:SER:CB	1:A:276:ILE:HD13	2.51	0.41
1:A:383:CYS:O	1:A:723:VAL:HA	2.21	0.41
1:A:437:CYS:O	1:A:517:LYS:HE2	2.20	0.41
2:B:214:GLN:HB2	2:B:251:ASN:HB2	2.03	0.41
1:A:920:ARG:HG2	1:A:920:ARG:H	1.71	0.41
1:A:947:LYS:HZ1	1:A:961:ASN:CB	2.34	0.41
2:B:139:GLN:CD	2:B:149:LYS:HD2	2.46	0.41
2:B:220:ALA:C	2:B:222:GLY:H	2.29	0.41
1:A:48:MET:HE3	1:A:48:MET:CA	2.30	0.41
1:A:945:ILE:HD11	1:A:1009:PHE:CA	2.39	0.41
2:B:143:LEU:O	2:B:150:PHE:CZ	2.74	0.41
1:A:255:SER:O	1:A:255:SER:OG	2.39	0.41
1:A:736:LYS:HA	1:A:736:LYS:HD2	1.79	0.41
2:B:197:PRO:HG2	2:B:224:TYR:HB2	2.03	0.41
1:A:883:ALA:HB1	2:B:66:ILE:HD13	2.03	0.40
2:B:70:THR:OG1	2:B:188:LYS:NZ	2.41	0.40
2:B:100:VAL:H	2:B:100:VAL:HG22	1.70	0.40
1:A:60:LEU:HD11	1:A:213:ARG:HG2	2.02	0.40
1:A:67:SER:HB3	1:A:71:GLY:N	2.36	0.40
1:A:744:GLY:N	1:A:759:LEU:O	2.50	0.40
1:A:807:VAL:HA	1:A:892:CYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HB2	1:A:278:ARG:HH12	1.86	0.40
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.73	0.40
1:A:777:ILE:O	1:A:781:LEU:HG	2.22	0.40
1:A:945:ILE:CG2	1:A:1012:ASP:OD2	2.69	0.40
1:A:631:ILE:HD12	1:A:631:ILE:H	1.85	0.40
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.61	0.40
1:A:697:MET:HG3	1:A:698:VAL:N	2.35	0.40
2:B:206:GLN:N	2:B:207:PRO:CD	2.85	0.40
1:A:710:ILE:O	1:A:711:VAL:C	2.64	0.40
1:A:786:ALA:HB2	1:A:858:LEU:HD11	2.03	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%)	936 (95%)	48 (5%)	0	100	100
2	B	259/261 (99%)	241 (93%)	18 (7%)	0	100	100
All	All	1243/1248 (100%)	1177 (95%)	66 (5%)	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%)	832 (100%)	1 (0%)	88	91
2	B	228/228 (100%)	228 (100%)	0	100	100
All	All	1061/1061 (100%)	1060 (100%)	1 (0%)	88	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	216	GLN
1	A	753	ASN
1	A	923	GLN
1	A	1029	GLN
2	B	214	GLN
2	B	251	ASN

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	3,1	8,11,12	6.06	3 (37%)	2,15,17	1.02	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	3,1	-	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	F3-BE	10.25	1.77	1.54
1	A	385	BFD	F1-BE	9.83	1.76	1.54
1	A	385	BFD	F2-BE	9.36	1.75	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	385	BFD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	301	2	14,14,15	1.03	2 (14%)	17,19,21	1.02	1 (5%)
6	NAG	B	302	2	14,14,15	0.77	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	B	303	2	14,14,15	0.35	0	17,19,21	0.61	0
5	J3C	A	1104	-	26,26,26	1.52	6 (23%)	29,39,39	2.27	9 (31%)

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	301	2	-	0/6/23/26	0/1/1/1
6	NAG	B	302	2	-	1/6/23/26	0/1/1/1
6	NAG	B	303	2	-	2/6/23/26	0/1/1/1
5	J3C	A	1104	-	-	4/4/20/20	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	J3C	C5-N1	-4.03	1.34	1.39
6	B	301	NAG	C1-C2	2.82	1.56	1.52
6	B	301	NAG	O5-C1	2.52	1.47	1.43
5	A	1104	J3C	C8-N1	-2.46	1.34	1.39
5	A	1104	J3C	C2-C3	-2.33	1.40	1.45
5	A	1104	J3C	C1-N1	-2.26	1.34	1.38
5	A	1104	J3C	C12-N3	-2.24	1.44	1.46
5	A	1104	J3C	C1-C2	2.15	1.40	1.35
6	B	302	NAG	C1-C2	2.14	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1104	J3C	C7-C8-N1	6.81	108.95	105.31
5	A	1104	J3C	C5-N2-C7	5.99	108.38	105.74
5	A	1104	J3C	C9-C7-N2	3.23	125.80	119.32
5	A	1104	J3C	C10-C8-C7	-3.12	124.92	131.23
6	B	302	NAG	C1-O5-C5	3.08	116.31	112.19
5	A	1104	J3C	O2-C11-C6	-2.70	104.29	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	NAG	C1-O5-C5	2.52	115.56	112.19
5	A	1104	J3C	C8-C7-N2	-2.36	106.00	110.24
5	A	1104	J3C	O2-C11-C12	2.22	113.46	108.98
5	A	1104	J3C	C13-C12-N3	-2.20	107.27	110.86
5	A	1104	J3C	N1-C5-N2	-2.08	109.47	111.55

There are no chirality outliers.

All (7) torsion outliers are listed below:

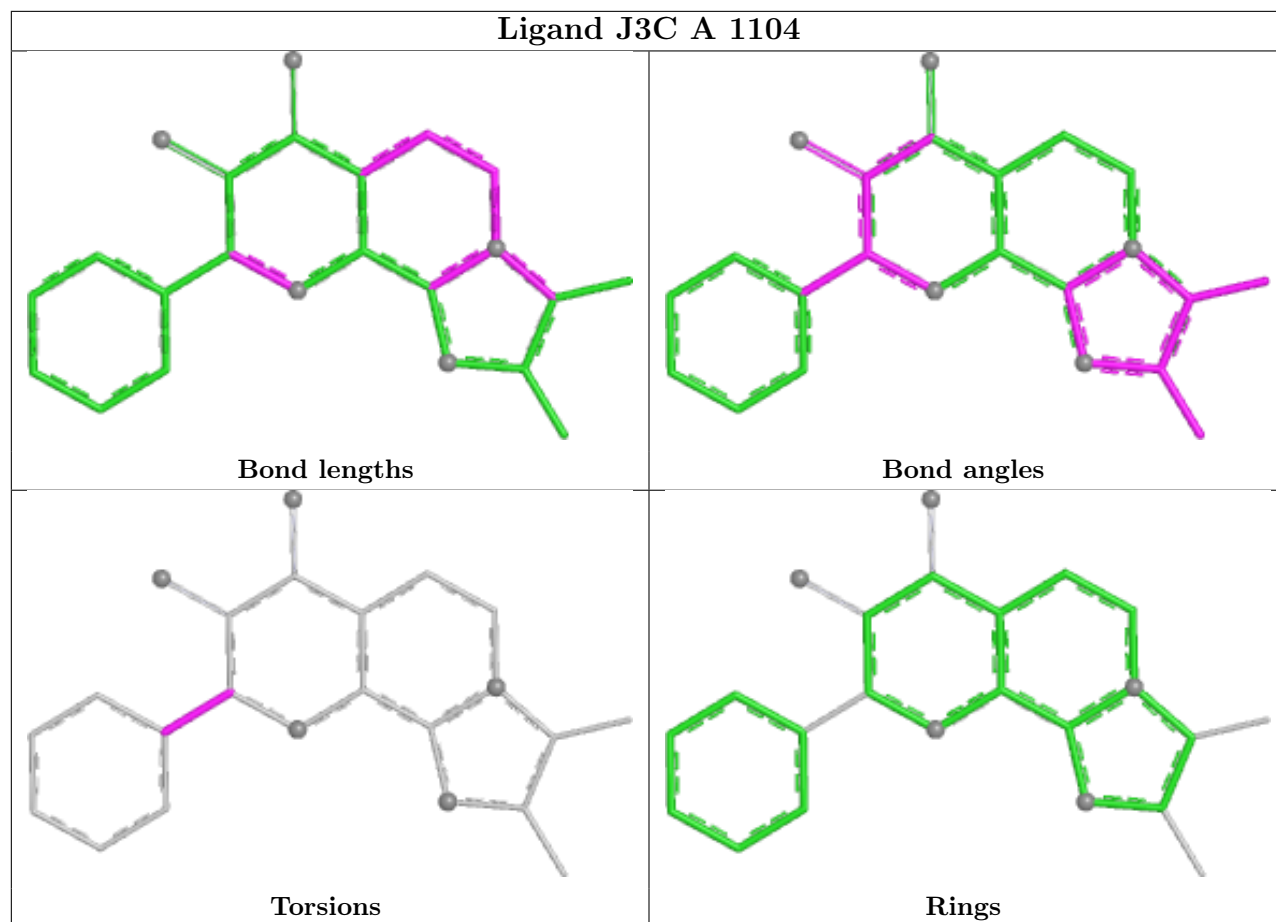
Mol	Chain	Res	Type	Atoms
6	B	303	NAG	O5-C5-C6-O6
6	B	303	NAG	C4-C5-C6-O6
5	A	1104	J3C	N3-C12-C13-C14
5	A	1104	J3C	N3-C12-C13-C18
5	A	1104	J3C	C11-C12-C13-C14
5	A	1104	J3C	C11-C12-C13-C18
6	B	302	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	NAG	1	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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	986/987 (99%)	0.03	40 (4%) 41 25	32, 70, 124, 213	0
2	B	261/261 (100%)	0.49	21 (8%) 18 12	58, 103, 165, 209	0
All	All	1247/1248 (99%)	0.13	61 (4%) 35 22	32, 76, 136, 213	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	GLU	6.8
1	A	174	VAL	6.5
1	A	173	LEU	5.3
2	B	242	ASN	5.1
2	B	229	PHE	4.8
1	A	50	ILE	4.5
1	A	599	SER	4.4
1	A	601	ILE	4.2
1	A	172	ASN	4.1
2	B	182	LYS	3.8
2	B	181	ILE	3.7
2	B	183	MET	3.6
1	A	906	ASP	3.6
2	B	241	SER	3.5
2	B	243	PRO	3.5
1	A	488	GLU	3.4
1	A	491	PHE	3.4
1	A	560	ARG	3.3
1	A	498	GLN	3.3
1	A	369	ASN	3.3
1	A	175	PRO	3.2
1	A	598	VAL	3.2
1	A	438	ASN	3.2
1	A	600	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	180	ILE	3.0
2	B	224	TYR	2.9
2	B	228	TYR	2.7
1	A	437	CYS	2.7
2	B	152	CYS	2.7
2	B	230	PRO	2.7
1	A	108	GLY	2.6
2	B	236	ALA	2.6
1	A	558	GLY	2.5
1	A	467	LYS	2.5
1	A	768	VAL	2.5
2	B	69	TYR	2.5
1	A	561	VAL	2.4
1	A	727	GLY	2.4
1	A	918	GLY	2.4
2	B	116	PHE	2.4
1	A	559	GLU	2.4
1	A	469	SER	2.4
1	A	555	GLY	2.3
2	B	237	GLN	2.3
2	B	87	ASP	2.3
1	A	332	PHE	2.3
1	A	1033	TYR	2.3
1	A	904	LEU	2.2
2	B	89	TYR	2.2
2	B	240	TYR	2.2
1	A	82	LEU	2.2
1	A	227	LEU	2.2
1	A	440	ALA	2.2
1	A	485	LYS	2.1
1	A	556	GLY	2.1
1	A	684	PRO	2.1
1	A	993	ILE	2.1
2	B	264	ILE	2.1
1	A	668	ASP	2.1
2	B	127	GLY	2.0
1	A	489	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	BFD	A	385	12/13	0.95	0.07	41,50,54,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

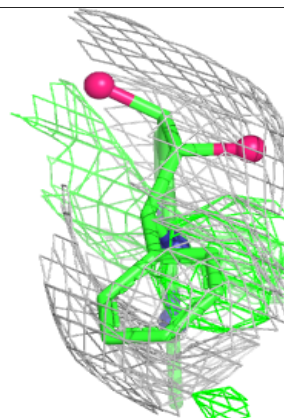
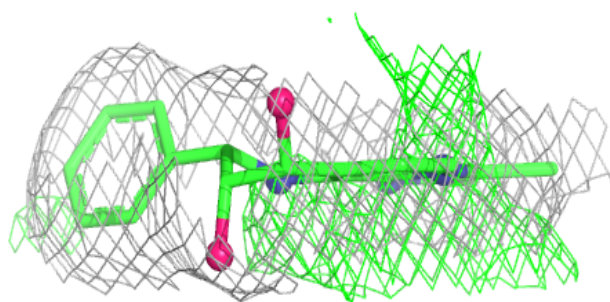
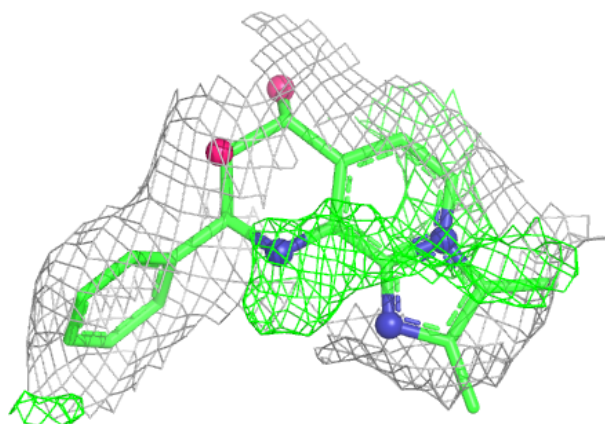
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	B	302	14/15	0.48	0.14	173,185,195,196	0
6	NAG	B	303	14/15	0.89	0.16	149,153,157,158	0
6	NAG	B	301	14/15	0.93	0.10	63,70,80,81	0
5	J3C	A	1104	23/23	0.95	0.12	68,79,84,90	0
4	RB	A	1103	1/1	0.97	0.04	79,79,79,79	0
3	MG	A	1101	1/1	0.98	0.11	53,53,53,53	0
4	RB	A	1102	1/1	0.99	0.08	83,83,83,83	0
4	RB	A	1105	1/1	0.99	0.11	97,97,97,97	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 1104:

$2mF_o-DF_c$ (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.