



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:45 AM UTC

PDB ID : 2OLE / pdb_00002ole
Title : Crystal Structure Of Human Dipeptidyl Peptidase IV (DPPIV) Complex With Cyclic Hydrazine Derivatives
Authors : Kim, S.S.; Ahn, J.H.; Lee, J.O.
Deposited on : 2007-01-19
Resolution : 2.40 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

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

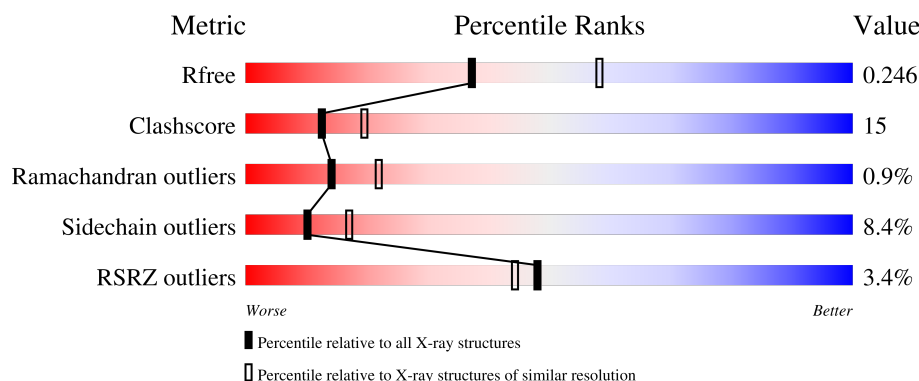
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

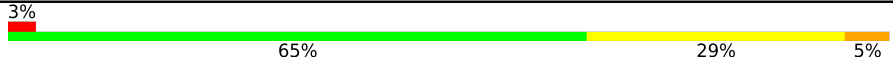
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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.

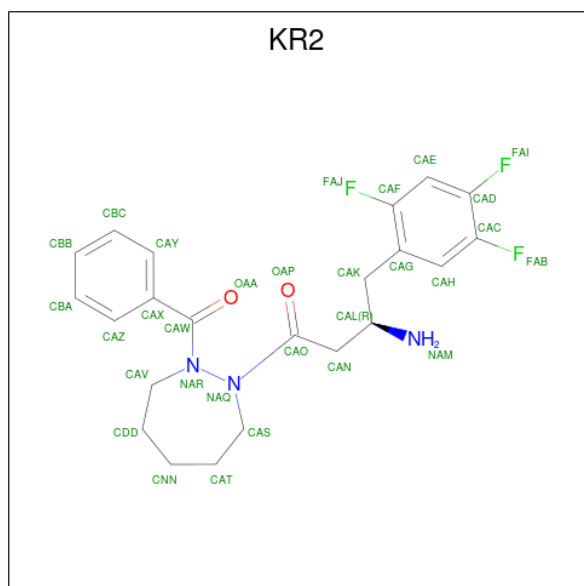
Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total 5948	C 3816	N 980	O 1126	S 26	0	0	0
1	B	728	Total 5964	C 3827	N 982	O 1129	S 26	0	0	0

- Molecule 2 is (2R)-4-(2-BENZOYL-1,2-DIAZEPAN-1-YL)-4-OXO-1-(2,4,5-TRIFLUOROPHENYL)BUTAN-2-AMINE (CCD ID: KR2) (formula: $C_{22}H_{24}F_3N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 22	F 3	N 3	O 2	0	0
2	B	1	Total 30	C 22	F 3	N 3	O 2	0	0

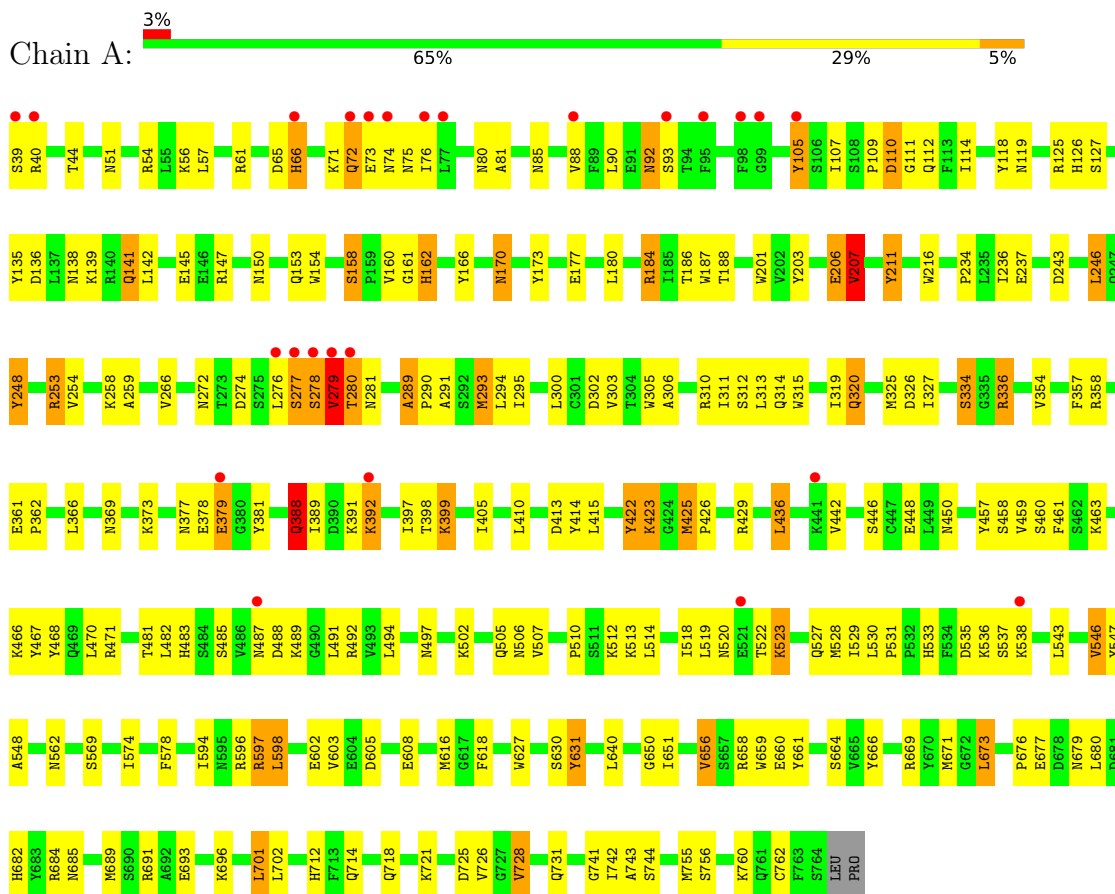
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total 227	O 227	0	0
3	B	311	Total 311	O 311	0	0

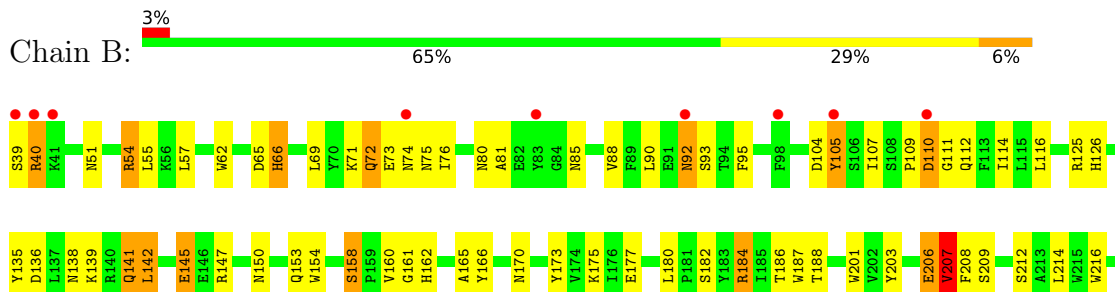
3 Residue-property plots

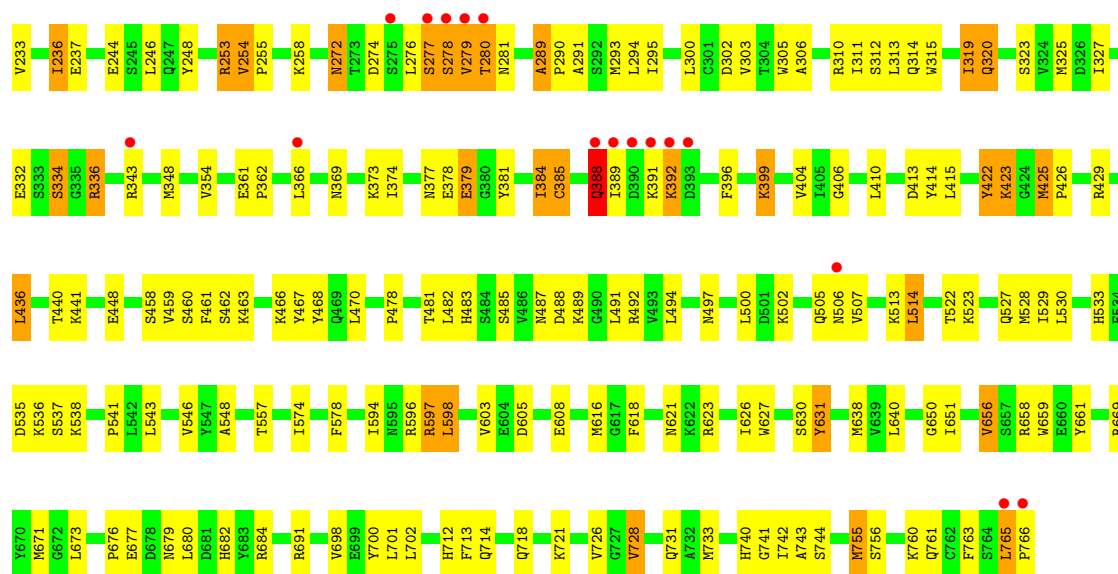
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.86Å 126.55Å 112.14Å 90.00° 99.64° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	81.6 (20.00-2.40) 88.1 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.38Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.254 0.203 , 0.246	Depositor DCC
R_{free} test set	5731 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12510	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: KR2

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	0.87	1/6119 (0.0%)	1.18	40/8321 (0.5%)
1	B	0.88	4/6136 (0.1%)	1.18	45/8344 (0.5%)
All	All	0.88	5/12255 (0.0%)	1.18	85/16665 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	755	MET	SD-CE	-7.79	1.60	1.79
1	B	348	MET	SD-CE	7.65	1.98	1.79
1	B	733	MET	SD-CE	5.66	1.93	1.79
1	A	279	VAL	CA-CB	5.45	1.61	1.54
1	B	638	MET	SD-CE	5.19	1.92	1.79

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	LYS	N-CA-C	9.70	121.85	111.28
1	B	656	VAL	N-CA-C	-9.46	96.49	109.55
1	A	656	VAL	N-CA-C	-9.19	96.87	109.55
1	B	392	LYS	N-CA-C	8.92	120.61	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	GLY	N-CA-C	-8.19	104.56	115.21
1	A	158	SER	N-CA-C	-7.77	98.72	110.07
1	A	206	GLU	CA-C-N	-7.74	115.26	123.08
1	A	206	GLU	C-N-CA	-7.74	115.26	123.08
1	B	206	GLU	N-CA-C	7.69	122.98	112.90
1	A	150	ASN	N-CA-C	-7.58	100.31	110.55
1	B	463	LYS	N-CA-C	7.47	120.07	111.11
1	B	150	ASN	N-CA-C	-7.43	100.52	110.55
1	B	458	SER	N-CA-C	-7.40	98.06	109.24
1	A	378	GLU	N-CA-C	-7.27	103.08	112.23
1	A	111	GLY	N-CA-C	-7.25	105.32	115.32
1	A	458	SER	N-CA-C	-7.17	98.42	109.24
1	A	388	GLN	N-CA-C	-7.15	97.58	109.24
1	B	158	SER	N-CA-C	-7.12	99.67	110.07
1	A	207	VAL	N-CA-C	6.95	117.54	111.56
1	B	320	GLN	N-CA-C	6.95	122.65	113.20
1	A	320	GLN	N-CA-C	6.94	122.63	113.20
1	B	207	VAL	N-CA-C	6.91	117.08	111.62
1	B	485	SER	N-CA-C	6.84	119.57	111.71
1	A	463	LYS	N-CA-C	6.78	119.54	111.33
1	B	319	ILE	N-CA-C	-6.72	97.25	107.73
1	A	319	ILE	N-CA-C	-6.66	97.34	107.73
1	B	378	GLU	N-CA-C	-6.45	104.10	112.23
1	B	110	ASP	N-CA-C	6.43	118.29	111.28
1	A	162	HIS	N-CA-C	6.31	118.49	110.61
1	A	485	SER	N-CA-C	6.29	118.95	111.71
1	B	206	GLU	CA-C-N	-6.27	116.51	123.16
1	B	206	GLU	C-N-CA	-6.27	116.51	123.16
1	B	385	CYS	CA-CB-SG	6.16	128.56	114.40
1	A	206	GLU	N-CA-C	6.15	120.96	112.90
1	B	388	GLN	N-CA-C	-6.14	99.23	109.24
1	B	300	LEU	N-CA-C	-6.12	99.23	108.96
1	B	201	TRP	N-CA-C	6.08	118.41	111.11
1	B	109	PRO	CA-C-N	5.97	128.28	120.28
1	B	109	PRO	C-N-CA	5.97	128.28	120.28
1	B	744	SER	N-CA-C	-5.95	102.64	110.43
1	A	548	ALA	N-CA-C	5.94	119.84	112.24
1	A	109	PRO	CA-C-N	5.88	128.16	120.28
1	A	109	PRO	C-N-CA	5.88	128.16	120.28
1	B	743	ALA	N-CA-C	5.85	121.14	113.30
1	A	248	TYR	CA-C-N	5.84	125.80	119.78
1	A	248	TYR	C-N-CA	5.84	125.80	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ILE	N-CA-C	-5.80	98.68	107.73
1	A	358	ARG	N-CA-C	-5.80	102.91	108.13
1	A	300	LEU	N-CA-C	-5.79	99.76	108.96
1	B	236	ILE	N-CA-C	-5.62	100.32	108.87
1	A	354	VAL	CB-CA-C	-5.62	103.20	110.84
1	A	201	TRP	N-CA-C	5.56	117.78	111.11
1	A	743	ALA	N-CA-C	5.56	120.75	113.30
1	B	188	THR	N-CA-C	5.54	120.16	113.17
1	B	110	ASP	CB-CA-C	-5.54	101.60	110.79
1	B	659	TRP	N-CA-C	5.48	118.01	111.71
1	B	384	ILE	CA-C-N	-5.46	114.76	122.94
1	B	384	ILE	C-N-CA	-5.46	114.76	122.94
1	B	233	VAL	CA-C-N	-5.45	114.98	120.21
1	B	233	VAL	C-N-CA	-5.45	114.98	120.21
1	A	664	SER	N-CA-C	5.43	116.88	111.07
1	A	725	ASP	N-CA-C	5.40	117.92	111.71
1	A	659	TRP	N-CA-C	5.38	118.64	111.75
1	B	623	ARG	N-CA-C	5.34	116.86	109.54
1	A	422	TYR	N-CA-C	5.33	118.20	110.42
1	B	165	ALA	N-CA-C	-5.33	100.34	109.24
1	B	621	ASN	CB-CA-C	-5.32	101.91	110.74
1	A	529	ILE	N-CA-C	-5.29	99.47	107.73
1	A	110	ASP	CB-CA-C	-5.24	102.10	110.79
1	A	562	ASN	N-CA-C	5.23	115.28	108.07
1	A	266	VAL	N-CA-C	5.22	117.38	108.86
1	B	548	ALA	N-CA-C	5.19	118.89	112.24
1	B	354	VAL	CB-CA-C	-5.18	103.79	110.84
1	A	631	TYR	N-CA-C	-5.18	105.81	111.82
1	A	546	VAL	N-CA-C	5.17	117.28	108.86
1	B	541	PRO	N-CA-C	-5.16	103.67	111.41
1	B	631	TYR	N-CA-C	-5.12	105.82	111.71
1	B	422	TYR	N-CA-C	5.10	117.73	110.24
1	B	698	VAL	N-CA-C	5.09	116.23	108.80
1	A	188	THR	N-CA-C	5.08	119.57	113.17
1	B	142	LEU	N-CA-C	-5.07	100.47	108.73
1	A	744	SER	N-CA-C	-5.06	103.80	110.43
1	A	293	MET	N-CA-C	-5.05	106.80	113.12
1	B	332	GLU	N-CA-C	5.05	117.44	111.33
1	B	546	VAL	N-CA-C	5.04	117.07	108.86

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	TYR	Sidechain
1	B	700	TYR	Sidechain

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	5948	0	5667	176	0
1	B	5964	0	5685	183	0
2	A	30	0	24	6	0
2	B	30	0	24	5	0
3	A	227	0	0	16	0
3	B	311	0	0	15	0
All	All	12510	0	11400	357	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 15.

All (357) 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:392:LYS:HE3	3:A:1004:HOH:O	1.55	1.02
2:B:1002:KR2:OAA	2:B:1002:KR2:HAS2	1.66	0.93
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.51	0.92
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.05	0.87
2:A:1001:KR2:OAA	2:A:1001:KR2:HAS2	1.74	0.86
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.05	0.86
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.56	0.86
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.59	0.82
1:B:280:THR:HG22	1:B:281:ASN:H	1.44	0.81
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.60	0.80
1:A:280:THR:HG22	1:A:281:ASN:H	1.46	0.80
1:B:92:ASN:HD22	1:B:93:SER:H	1.29	0.79
1:A:92:ASN:HD22	1:A:93:SER:H	1.29	0.78
1:B:114:ILE:HG22	1:B:135:TYR:HB3	1.65	0.77
1:B:325:MET:HE2	1:B:327:ILE:HD11	1.68	0.76
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.67	0.75
1:B:110:ASP:HB3	1:B:112:GLN:HG3	1.67	0.75
1:B:76:ILE:HG22	1:B:90:LEU:HB3	1.71	0.73
1:A:334:SER:OG	1:A:336:ARG:HD3	1.87	0.73
1:B:272:ASN:HD22	1:B:274:ASP:H	1.34	0.73
1:A:110:ASP:HB3	1:A:112:GLN:HG3	1.69	0.73
1:B:76:ILE:HD12	1:B:105:TYR:CZ	2.23	0.72
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.24	0.72
1:A:76:ILE:HD12	1:A:105:TYR:CZ	2.24	0.72
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.88	0.72
1:B:334:SER:OG	1:B:336:ARG:HD3	1.88	0.72
1:A:336:ARG:HH11	1:A:336:ARG:HB3	1.55	0.71
1:A:76:ILE:HG22	1:A:90:LEU:HB3	1.70	0.71
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.71	0.71
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.88	0.71
1:B:336:ARG:HB3	1:B:336:ARG:HH11	1.54	0.70
1:B:289:ALA:HB1	1:B:290:PRO:C	2.15	0.70
1:B:765:LEU:HB3	1:B:766:PRO:OXT	1.92	0.70
1:A:762:CYS:HB2	3:A:1110:HOH:O	1.91	0.69
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.28	0.69
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.75	0.69
1:B:369:ASN:HA	1:B:389:ILE:HD13	1.75	0.69
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.28	0.68
1:B:691:ARG:NH1	3:B:1106:HOH:O	2.25	0.68
1:B:487:ASN:HB2	3:B:1183:HOH:O	1.92	0.67
2:B:1002:KR2:OAA	2:B:1002:KR2:CAS	2.36	0.67
1:B:528:MET:HE2	1:B:530:LEU:HD21	1.76	0.67
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.31	0.66
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.94	0.66
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.79	0.65
1:B:206:GLU:CD	2:B:1002:KR2:HAM1	2.05	0.65
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.78	0.65
1:B:272:ASN:ND2	1:B:274:ASP:H	1.95	0.65
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.32	0.65
1:A:289:ALA:HB1	1:A:290:PRO:C	2.22	0.64
2:A:1001:KR2:OAA	2:A:1001:KR2:CAS	2.40	0.64
1:A:289:ALA:CB	1:A:290:PRO:CA	2.76	0.64
1:A:314:GLN:HE22	1:A:373:LYS:NZ	1.96	0.63
1:B:596:ARG:O	1:B:597:ARG:HD2	1.99	0.63
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.80	0.63
1:B:314:GLN:HE22	1:B:373:LYS:NZ	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG12	1:B:114:ILE:HG13	1.81	0.63
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.47	0.62
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.98	0.62
1:B:388:GLN:HB2	1:B:391:LYS:HB3	1.81	0.62
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.82	0.62
1:A:187:TRP:HZ3	3:A:1190:HOH:O	1.83	0.62
1:A:627:TRP:CE3	1:A:755:MET:HE1	2.35	0.62
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.35	0.61
1:B:377:ASN:HB2	1:B:381:TYR:H	1.66	0.61
1:B:289:ALA:CB	1:B:290:PRO:CA	2.75	0.61
1:B:289:ALA:CB	1:B:290:PRO:HA	2.29	0.61
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.00	0.61
1:A:528:MET:HE3	1:A:574:ILE:HG21	1.83	0.61
1:B:441:LYS:HE3	3:B:1192:HOH:O	2.00	0.61
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.82	0.60
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.32	0.60
1:A:57:LEU:HD23	3:A:1061:HOH:O	2.01	0.60
1:B:399:LYS:HD2	1:B:399:LYS:C	2.27	0.59
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.38	0.59
1:A:651:ILE:CG2	1:A:755:MET:HE3	2.29	0.59
1:A:289:ALA:CB	1:A:290:PRO:HA	2.31	0.59
1:A:377:ASN:HB2	1:A:381:TYR:H	1.66	0.59
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.38	0.59
1:A:596:ARG:O	1:A:597:ARG:HD2	2.02	0.58
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.86	0.58
1:A:369:ASN:HA	1:A:389:ILE:HD13	1.86	0.58
1:A:533:HIS:N	1:A:533:HIS:CD2	2.71	0.58
1:B:81:ALA:O	1:B:492:ARG:NH2	2.36	0.58
1:B:293:MET:HG2	1:B:315:TRP:HB3	1.86	0.58
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.49	0.58
1:B:314:GLN:HE22	1:B:373:LYS:HZ3	1.50	0.58
1:A:450:ASN:HB2	3:A:1083:HOH:O	2.04	0.57
1:A:81:ALA:O	1:A:492:ARG:NH2	2.37	0.57
1:A:272:ASN:HD22	1:A:274:ASP:H	1.52	0.57
1:A:44:THR:HB	3:A:1137:HOH:O	2.03	0.57
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.51	0.57
1:A:325:MET:CE	1:A:327:ILE:HD11	2.35	0.57
1:B:184:ARG:HD3	1:B:186:THR:O	2.04	0.57
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.40	0.57
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.02	0.57
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HE3	1:A:105:TYR:HE1	1.71	0.56
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.35	0.56
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.40	0.56
1:B:272:ASN:HD22	1:B:272:ASN:C	2.13	0.56
1:B:533:HIS:N	1:B:533:HIS:CD2	2.74	0.56
1:B:677:GLU:CD	1:B:677:GLU:H	2.14	0.56
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.40	0.55
1:A:399:LYS:HD2	1:A:399:LYS:C	2.31	0.55
1:A:65:ASP:HB3	1:A:66:HIS:CE1	2.42	0.54
1:A:535:ASP:OD2	1:A:537:SER:HB3	2.05	0.54
1:A:731:GLN:NE2	1:B:731:GLN:NE2	2.55	0.54
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.07	0.54
1:A:276:LEU:O	1:A:278:SER:N	2.40	0.54
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.89	0.54
1:B:596:ARG:C	1:B:597:ARG:HD2	2.32	0.54
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.08	0.54
1:A:505:GLN:HB3	3:A:1220:HOH:O	2.06	0.54
1:A:677:GLU:H	1:A:677:GLU:CD	2.16	0.54
1:B:323:SER:HB2	3:B:1124:HOH:O	2.08	0.54
1:A:184:ARG:HD3	1:A:186:THR:O	2.07	0.53
1:A:105:TYR:N	1:A:105:TYR:CD1	2.77	0.53
1:A:535:ASP:CG	1:A:537:SER:HB3	2.34	0.53
1:B:154:TRP:O	1:B:166:TYR:HA	2.08	0.53
1:A:482:LEU:HB2	1:A:494:LEU:HD11	1.91	0.53
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.05	0.53
1:B:139:LYS:HG3	1:B:141:GLN:HB2	1.89	0.53
1:B:630:SER:OG	2:B:1002:KR2:CAE	2.57	0.53
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.08	0.53
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.92	0.53
1:A:277:SER:O	1:A:278:SER:HB3	2.09	0.52
1:B:92:ASN:HD22	1:B:93:SER:N	2.05	0.52
1:A:105:TYR:N	1:A:105:TYR:HD1	2.08	0.52
1:A:107:ILE:HG12	1:A:114:ILE:HG13	1.91	0.52
1:B:276:LEU:O	1:B:278:SER:N	2.42	0.52
1:A:206:GLU:CD	2:A:1001:KR2:HAM1	2.16	0.51
1:B:760:LYS:HA	1:B:765:LEU:CD1	2.40	0.51
1:A:71:LYS:HB2	3:A:1199:HOH:O	2.10	0.51
1:A:388:GLN:HB2	1:A:391:LYS:HB3	1.92	0.51
1:B:277:SER:O	1:B:278:SER:HB3	2.10	0.51
1:B:325:MET:CE	1:B:327:ILE:HD11	2.39	0.51
1:A:72:GLN:O	1:A:74:ASN:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:O	1:B:74:ASN:N	2.41	0.51
1:B:528:MET:CE	1:B:530:LEU:HD21	2.40	0.51
1:A:535:ASP:C	1:A:537:SER:H	2.16	0.51
1:B:760:LYS:HA	1:B:765:LEU:HD13	1.93	0.51
1:B:466:LYS:HG2	1:B:467:TYR:CE2	2.45	0.51
1:B:651:ILE:CG2	1:B:755:MET:HE3	2.35	0.51
1:A:596:ARG:C	1:A:597:ARG:HD2	2.36	0.51
1:B:483:HIS:HD2	3:B:1142:HOH:O	1.94	0.51
1:A:691:ARG:NH1	3:A:1045:HOH:O	2.43	0.50
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.93	0.50
1:A:528:MET:CE	1:A:530:LEU:HD21	2.41	0.50
1:A:630:SER:OG	2:A:1001:KR2:CAE	2.59	0.50
1:A:731:GLN:NE2	1:B:731:GLN:HE22	2.09	0.50
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.12	0.50
1:B:429:ARG:NH2	3:B:1019:HOH:O	2.44	0.50
1:B:756:SER:O	1:B:760:LYS:HG3	2.11	0.50
1:A:92:ASN:HD22	1:A:93:SER:N	2.04	0.50
1:A:314:GLN:HE22	1:A:373:LYS:HZ3	1.60	0.50
1:A:487:ASN:O	1:A:488:ASP:HB2	2.12	0.49
1:B:65:ASP:HB3	1:B:66:HIS:CE1	2.48	0.49
1:A:160:VAL:HG12	1:A:161:GLY:N	2.27	0.49
1:A:76:ILE:HD12	1:A:105:TYR:CE2	2.46	0.49
1:A:512:LYS:HD3	3:A:1149:HOH:O	2.11	0.49
1:B:76:ILE:HB	1:B:105:TYR:OH	2.12	0.49
1:B:528:MET:HE3	1:B:574:ILE:HG21	1.94	0.49
1:A:731:GLN:HE22	1:B:731:GLN:NE2	2.10	0.49
1:B:105:TYR:N	1:B:105:TYR:CD1	2.80	0.49
1:B:170:ASN:N	1:B:170:ASN:HD22	2.10	0.49
1:A:74:ASN:CB	1:A:92:ASN:HB3	2.43	0.48
1:B:105:TYR:N	1:B:105:TYR:HD1	2.11	0.48
1:B:306:ALA:HB3	1:B:310:ARG:HB3	1.95	0.48
1:A:272:ASN:ND2	1:A:274:ASP:H	2.11	0.48
1:B:392:LYS:HD3	3:B:1058:HOH:O	2.13	0.48
1:B:513:LYS:O	1:B:527:GLN:HA	2.13	0.48
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.94	0.48
1:A:272:ASN:HD22	1:A:272:ASN:C	2.21	0.48
1:B:71:LYS:HE3	1:B:105:TYR:HE1	1.77	0.48
1:A:718:GLN:HE22	1:A:721:LYS:HZ1	1.60	0.48
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.14	0.48
1:B:391:LYS:HG3	3:B:1013:HOH:O	2.13	0.48
1:A:177:GLU:CG	1:A:180:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:HB3	3:B:1124:HOH:O	2.12	0.48
1:A:673:LEU:HD21	3:A:1116:HOH:O	2.14	0.48
1:B:57:LEU:HD23	3:B:1242:HOH:O	2.13	0.48
1:B:160:VAL:HG12	1:B:161:GLY:N	2.28	0.48
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.96	0.48
1:B:535:ASP:C	1:B:537:SER:H	2.21	0.48
1:A:92:ASN:N	1:A:92:ASN:ND2	2.61	0.47
1:A:253:ARG:NH2	1:B:253:ARG:NH2	2.61	0.47
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.49	0.47
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.14	0.47
1:A:712:HIS:C	1:A:714:GLN:N	2.72	0.47
1:A:518:ILE:O	1:A:519:LEU:HD23	2.14	0.47
1:B:377:ASN:HB3	1:B:379:GLU:H	1.78	0.47
1:A:415:LEU:HD23	1:A:415:LEU:C	2.39	0.47
1:B:669:ARG:NH1	3:B:1131:HOH:O	2.48	0.47
1:A:246:LEU:HD13	1:A:248:TYR:O	2.15	0.47
1:A:466:LYS:HG2	1:A:467:TYR:CE2	2.50	0.47
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.50	0.47
1:B:415:LEU:C	1:B:415:LEU:HD23	2.39	0.47
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.96	0.47
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.96	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.97	0.46
1:B:92:ASN:N	1:B:92:ASN:ND2	2.63	0.46
1:B:487:ASN:O	1:B:488:ASP:HB2	2.13	0.46
1:B:177:GLU:CG	1:B:180:LEU:HD22	2.45	0.46
1:A:74:ASN:C	1:A:92:ASN:HB3	2.40	0.46
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.50	0.46
1:B:305:TRP:CZ2	1:B:311:ILE:HD12	2.50	0.46
1:B:741:GLY:O	1:B:742:ILE:C	2.58	0.46
1:A:357:PHE:CD2	2:A:1001:KR2:HDD2	2.51	0.46
1:A:377:ASN:HB3	1:A:379:GLU:H	1.81	0.46
1:A:528:MET:HE1	1:A:618:PHE:CE1	2.50	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.59	0.46
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.50	0.46
1:A:442:VAL:O	1:A:442:VAL:HG13	2.15	0.46
1:B:214:LEU:HD12	1:B:214:LEU:O	2.16	0.46
1:B:440:THR:O	1:B:440:THR:HG22	2.16	0.46
1:B:598:LEU:HB2	1:B:671:MET:SD	2.56	0.46
1:A:756:SER:O	1:A:760:LYS:HG3	2.17	0.45
1:B:153:GLN:HE22	1:B:170:ASN:HD21	1.63	0.45
1:B:377:ASN:HB2	1:B:381:TYR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:HIS:C	1:B:714:GLN:N	2.73	0.45
1:B:289:ALA:HA	1:B:294:LEU:HG	1.98	0.45
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.52	0.45
1:A:598:LEU:HG	1:A:631:TYR:OH	2.16	0.45
1:A:92:ASN:ND2	1:A:92:ASN:H	2.14	0.45
1:A:535:ASP:C	1:A:537:SER:N	2.75	0.45
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.33	0.45
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.51	0.45
1:B:765:LEU:HB2	1:B:766:PRO:HA	1.98	0.45
1:B:92:ASN:ND2	1:B:93:SER:H	2.07	0.45
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.52	0.45
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.74	0.45
1:B:578:PHE:HE2	1:B:605:ASP:HB3	1.82	0.45
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.52	0.44
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.53	0.44
1:B:425:MET:HA	1:B:426:PRO:HD2	1.87	0.44
1:B:237:GLU:HG2	1:B:253:ARG:HB3	1.99	0.44
1:B:598:LEU:HG	1:B:631:TYR:OH	2.18	0.44
1:A:277:SER:O	1:A:278:SER:CB	2.65	0.44
1:A:578:PHE:HE2	1:A:605:ASP:HB3	1.83	0.44
1:B:369:ASN:C	1:B:389:ILE:HG23	2.43	0.44
1:A:110:ASP:HB3	1:A:112:GLN:H	1.83	0.44
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.18	0.44
1:A:689:MET:HE3	1:B:244:GLU:HG3	1.99	0.44
1:B:92:ASN:ND2	1:B:92:ASN:H	2.16	0.44
1:B:535:ASP:CG	1:B:537:SER:HB3	2.43	0.44
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.53	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.98	0.44
1:B:76:ILE:HD12	1:B:105:TYR:CE2	2.52	0.44
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.86	0.44
1:A:691:ARG:NH2	3:A:1005:HOH:O	2.36	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.43
1:B:74:ASN:C	1:B:92:ASN:HB3	2.43	0.43
1:A:502:LYS:O	1:A:505:GLN:HG2	2.18	0.43
1:A:154:TRP:O	1:A:166:TYR:HA	2.18	0.43
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.48	0.43
1:A:170:ASN:N	1:A:170:ASN:HD22	2.15	0.43
1:A:314:GLN:NE2	1:A:373:LYS:NZ	2.66	0.43
1:A:459:VAL:HG22	1:A:460:SER:N	2.34	0.43
1:A:666:TYR:CD2	2:A:1001:KR2:NAM	2.86	0.43
1:B:254:VAL:HA	1:B:255:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.01	0.43
1:B:391:LYS:HE3	1:B:391:LYS:HB2	1.85	0.43
1:B:528:MET:HE1	1:B:618:PHE:CE1	2.54	0.43
1:A:61:ARG:HH22	1:A:107:ILE:H	1.66	0.43
1:A:312:SER:O	1:A:313:LEU:HD12	2.18	0.43
1:A:76:ILE:CG2	1:A:90:LEU:HB3	2.46	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.19	0.43
1:B:291:ALA:O	1:B:295:ILE:HG23	2.19	0.43
1:B:277:SER:O	1:B:278:SER:CB	2.66	0.43
1:A:39:SER:N	3:A:1183:HOH:O	2.52	0.43
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.01	0.43
1:B:312:SER:O	1:B:313:LEU:HD12	2.18	0.43
1:B:336:ARG:NH1	3:B:1218:HOH:O	2.52	0.43
1:A:80:ASN:HB3	1:A:85:ASN:OD1	2.19	0.43
1:A:107:ILE:CG1	1:A:114:ILE:HG13	2.48	0.43
1:A:173:TYR:CZ	1:A:184:ARG:HG3	2.53	0.43
1:A:523:LYS:H	1:A:523:LYS:HG2	1.69	0.43
1:B:74:ASN:CB	1:B:92:ASN:HB3	2.47	0.43
1:B:76:ILE:O	1:B:76:ILE:CG2	2.66	0.43
1:B:76:ILE:CG2	1:B:90:LEU:HB3	2.46	0.43
1:A:671:MET:HE1	1:A:682:HIS:HD2	1.84	0.42
1:B:110:ASP:HB3	1:B:112:GLN:H	1.82	0.42
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.54	0.42
1:B:482:LEU:HB2	1:B:494:LEU:HD11	2.01	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.01	0.42
1:A:305:TRP:CZ2	1:A:311:ILE:HD12	2.53	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.00	0.42
1:B:594:ILE:HD12	1:B:598:LEU:HD12	2.00	0.42
1:A:425:MET:HA	1:A:426:PRO:HD2	1.87	0.42
1:B:136:ASP:OD1	1:B:138:ASN:HB2	2.20	0.42
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.66	0.42
1:B:208:PHE:O	1:B:209:SER:C	2.62	0.42
1:B:319:ILE:HD13	1:B:319:ILE:HA	1.90	0.42
1:A:457:TYR:HA	1:A:471:ARG:O	2.19	0.42
1:B:413:ASP:O	1:B:436:LEU:HB2	2.19	0.42
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.64	0.42
1:A:489:LYS:HE3	1:A:491:LEU:HD23	2.01	0.42
1:A:594:ILE:HD12	1:A:598:LEU:HD12	2.01	0.42
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.50	0.42
1:B:92:ASN:HD22	1:B:92:ASN:N	2.17	0.42
1:B:158:SER:HA	1:B:216:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:GLU:OE2	1:A:696:LYS:HE2	2.20	0.42
1:B:175:LYS:NZ	1:B:182:SER:HB3	2.34	0.42
1:B:392:LYS:HE2	3:B:1236:HOH:O	2.19	0.42
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.42
1:A:127:SER:HB3	1:A:211:TYR:CG	2.54	0.42
1:A:243:ASP:HB3	3:A:1178:HOH:O	2.20	0.42
1:A:546:VAL:HG22	1:A:547:TYR:N	2.33	0.42
1:B:740:HIS:NE2	2:B:1002:KR2:HAE	2.35	0.42
1:A:76:ILE:HD11	3:A:1189:HOH:O	2.20	0.42
1:A:405:ILE:HG13	1:A:429:ARG:CD	2.50	0.42
1:B:763:PHE:HB2	1:B:765:LEU:HD12	2.02	0.42
1:A:289:ALA:HA	1:A:294:LEU:HG	2.02	0.41
1:B:145:GLU:HG2	3:B:1152:HOH:O	2.20	0.41
1:B:374:ILE:CD1	1:B:406:GLY:HA2	2.49	0.41
1:B:502:LYS:O	1:B:505:GLN:HG2	2.19	0.41
1:A:92:ASN:HD22	1:A:92:ASN:N	2.17	0.41
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.20	0.41
1:B:489:LYS:HE3	1:B:491:LEU:HD23	2.02	0.41
1:A:125:ARG:HD2	1:A:126:HIS:CE1	2.55	0.41
1:A:291:ALA:O	1:A:295:ILE:HG23	2.20	0.41
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.55	0.41
1:A:314:GLN:HE22	1:A:373:LYS:HZ1	1.63	0.41
1:A:377:ASN:HB2	1:A:381:TYR:N	2.32	0.41
1:A:520:ASN:ND2	3:A:1150:HOH:O	2.53	0.41
1:B:54:ARG:HE	1:B:54:ARG:HB2	1.65	0.41
1:A:502:LYS:HD2	1:A:502:LYS:HA	1.92	0.41
1:B:459:VAL:HG22	1:B:460:SER:N	2.35	0.41
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.96	0.41
1:B:104:ASP:OD1	1:B:105:TYR:N	2.53	0.41
1:A:118:TYR:O	1:A:119:ASN:HB2	2.21	0.41
1:A:528:MET:HE1	1:A:618:PHE:HE1	1.85	0.41
1:B:535:ASP:C	1:B:537:SER:N	2.79	0.41
1:A:237:GLU:HG2	1:A:253:ARG:HB3	2.03	0.41
1:A:602:GLU:OE2	1:A:602:GLU:N	2.50	0.41
1:A:651:ILE:HG23	1:A:701:LEU:HB3	2.02	0.41
1:B:388:GLN:HB3	3:B:1141:HOH:O	2.21	0.41
1:B:671:MET:HE1	1:B:682:HIS:CD2	2.56	0.41
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.21	0.41
1:A:640:LEU:HD11	1:A:650:GLY:HA3	2.03	0.40
1:B:314:GLN:NE2	1:B:373:LYS:HZ3	2.17	0.40
1:A:236:ILE:HG12	1:A:712:HIS:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HG13	1:A:398:THR:HG23	2.03	0.40
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.51	0.40
1:B:712:HIS:O	1:B:713:PHE:C	2.64	0.40
1:A:158:SER:HA	1:A:216:TRP:CD1	2.57	0.40
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.56	0.40
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.56	0.40
1:B:535:ASP:OD2	1:B:537:SER:HB3	2.22	0.40
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.57	0.40
1:A:513:LYS:HE3	1:A:530:LEU:HD11	2.03	0.40
1:B:39:SER:O	1:B:40:ARG:O	2.40	0.40
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.57	0.40
1:B:314:GLN:NE2	1:B:373:LYS:NZ	2.67	0.40
1:B:478:PRO:HB2	1:B:497:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	685 (95%)	33 (5%)	6 (1%)	16	25
1	B	726/728 (100%)	690 (95%)	29 (4%)	7 (1%)	12	20
All	All	1450/1456 (100%)	1375 (95%)	62 (4%)	13 (1%)	14	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	277	SER
1	A	278	SER
1	A	279	VAL
1	B	40	ARG

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Mol	Chain	Res	Type
1	B	277	SER
1	B	278	SER
1	B	279	VAL
1	B	765	LEU
1	A	73	GLU
1	A	289	ALA
1	B	289	ALA
1	B	73	GLU

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	651/653 (100%)	597 (92%)	54 (8%)	10	17
1	B	653/653 (100%)	598 (92%)	55 (8%)	10	17
All	All	1304/1306 (100%)	1195 (92%)	109 (8%)	10	17

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	54	ARG
1	A	66	HIS
1	A	72	GLN
1	A	75	ASN
1	A	88	VAL
1	A	92	ASN
1	A	105	TYR
1	A	141	GLN
1	A	142	LEU
1	A	145	GLU
1	A	147	ARG
1	A	170	ASN
1	A	184	ARG
1	A	207	VAL

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	279	VAL
1	A	280	THR
1	A	303	VAL
1	A	334	SER
1	A	336	ARG
1	A	361	GLU
1	A	362	PRO
1	A	366	LEU
1	A	379	GLU
1	A	388	GLN
1	A	399	LYS
1	A	410	LEU
1	A	423	LYS
1	A	425	MET
1	A	436	LEU
1	A	448	GLU
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	522	THR
1	A	523	LYS
1	A	536	LYS
1	A	538	LYS
1	A	543	LEU
1	A	597	ARG
1	A	598	LEU
1	A	603	VAL
1	A	608	GLU
1	A	616	MET
1	A	656	VAL
1	A	673	LEU
1	A	679	ASN
1	A	685	ASN
1	A	701	LEU
1	A	702	LEU
1	A	728	VAL
1	B	51	ASN
1	B	54	ARG
1	B	66	HIS

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	75	ASN
1	B	88	VAL
1	B	92	ASN
1	B	105	TYR
1	B	141	GLN
1	B	142	LEU
1	B	145	GLU
1	B	147	ARG
1	B	184	ARG
1	B	207	VAL
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	279	VAL
1	B	280	THR
1	B	303	VAL
1	B	334	SER
1	B	336	ARG
1	B	343	ARG
1	B	361	GLU
1	B	362	PRO
1	B	366	LEU
1	B	379	GLU
1	B	388	GLN
1	B	399	LYS
1	B	410	LEU
1	B	423	LYS
1	B	425	MET
1	B	436	LEU
1	B	448	GLU
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	522	THR
1	B	523	LYS
1	B	536	LYS
1	B	538	LYS
1	B	543	LEU
1	B	597	ARG
1	B	598	LEU

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Mol	Chain	Res	Type
1	B	603	VAL
1	B	608	GLU
1	B	616	MET
1	B	656	VAL
1	B	673	LEU
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	728	VAL
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	72	GLN
1	A	74	ASN
1	A	92	ASN
1	A	103	ASN
1	A	112	GLN
1	A	123	GLN
1	A	126	HIS
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	455	GLN
1	A	483	HIS
1	A	505	GLN
1	A	506	ASN
1	A	572	ASN
1	A	586	GLN
1	A	679	ASN
1	A	694	ASN
1	A	712	HIS
1	A	718	GLN
1	A	731	GLN
1	B	66	HIS
1	B	72	GLN
1	B	74	ASN
1	B	92	ASN

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	123	GLN
1	B	126	HIS
1	B	169	ASN
1	B	170	ASN
1	B	196	ASN
1	B	227	GLN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	344	GLN
1	B	345	HIS
1	B	430	ASN
1	B	455	GLN
1	B	483	HIS
1	B	505	GLN
1	B	506	ASN
1	B	533	HIS
1	B	572	ASN
1	B	586	GLN
1	B	679	ASN
1	B	694	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	KR2	B	1002	-	30,32,32	2.75	5 (16%)	32,44,44	2.70	8 (25%)
2	KR2	A	1001	-	30,32,32	2.76	5 (16%)	32,44,44	2.60	9 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KR2	B	1002	-	-	7/13/32/32	0/2/3/3
2	KR2	A	1001	-	-	6/13/32/32	0/2/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	KR2	OAA-CAW	10.50	1.43	1.22
2	A	1001	KR2	OAA-CAW	10.49	1.43	1.22
2	A	1001	KR2	CAK-CAG	-7.55	1.39	1.51
2	B	1002	KR2	CAK-CAG	-7.44	1.39	1.51
2	B	1002	KR2	OAP-CAO	6.12	1.36	1.23
2	A	1001	KR2	OAP-CAO	6.11	1.36	1.23
2	A	1001	KR2	CAW-NAR	3.08	1.47	1.37
2	B	1002	KR2	CAW-NAR	3.03	1.47	1.37
2	B	1002	KR2	CAX-CAW	2.30	1.53	1.50
2	A	1001	KR2	CAX-CAW	2.22	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	KR2	CAX-CAW-NAR	-10.10	100.53	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	KR2	CAX-CAW-NAR	-8.55	103.28	118.44
2	A	1001	KR2	OAA-CAW-CAX	-5.93	108.53	120.29
2	A	1001	KR2	OAA-CAW-NAR	-5.63	111.68	120.25
2	B	1002	KR2	OAA-CAW-NAR	-5.15	112.40	120.25
2	A	1001	KR2	CAV-NAR-CAW	-5.09	109.30	119.16
2	B	1002	KR2	CAV-NAR-CAW	-5.00	109.47	119.16
2	B	1002	KR2	OAA-CAW-CAX	-4.93	110.52	120.29
2	B	1002	KR2	CAK-CAG-CAF	-3.10	118.27	122.45
2	B	1002	KR2	CAE-CAF-CAG	-2.99	119.15	123.76
2	A	1001	KR2	CAE-CAF-CAG	-2.85	119.36	123.76
2	B	1002	KR2	CAF-CAE-CAD	2.77	121.88	117.22
2	A	1001	KR2	FAJ-CAF-CAG	2.70	122.46	117.96
2	A	1001	KR2	OAP-CAO-CAN	-2.55	117.30	122.07
2	A	1001	KR2	CAF-CAE-CAD	2.53	121.49	117.22
2	B	1002	KR2	FAJ-CAF-CAG	2.31	121.81	117.96
2	A	1001	KR2	CAH-CAG-CAF	2.06	118.81	116.54

There are no chirality outliers.

All (13) torsion outliers are listed below:

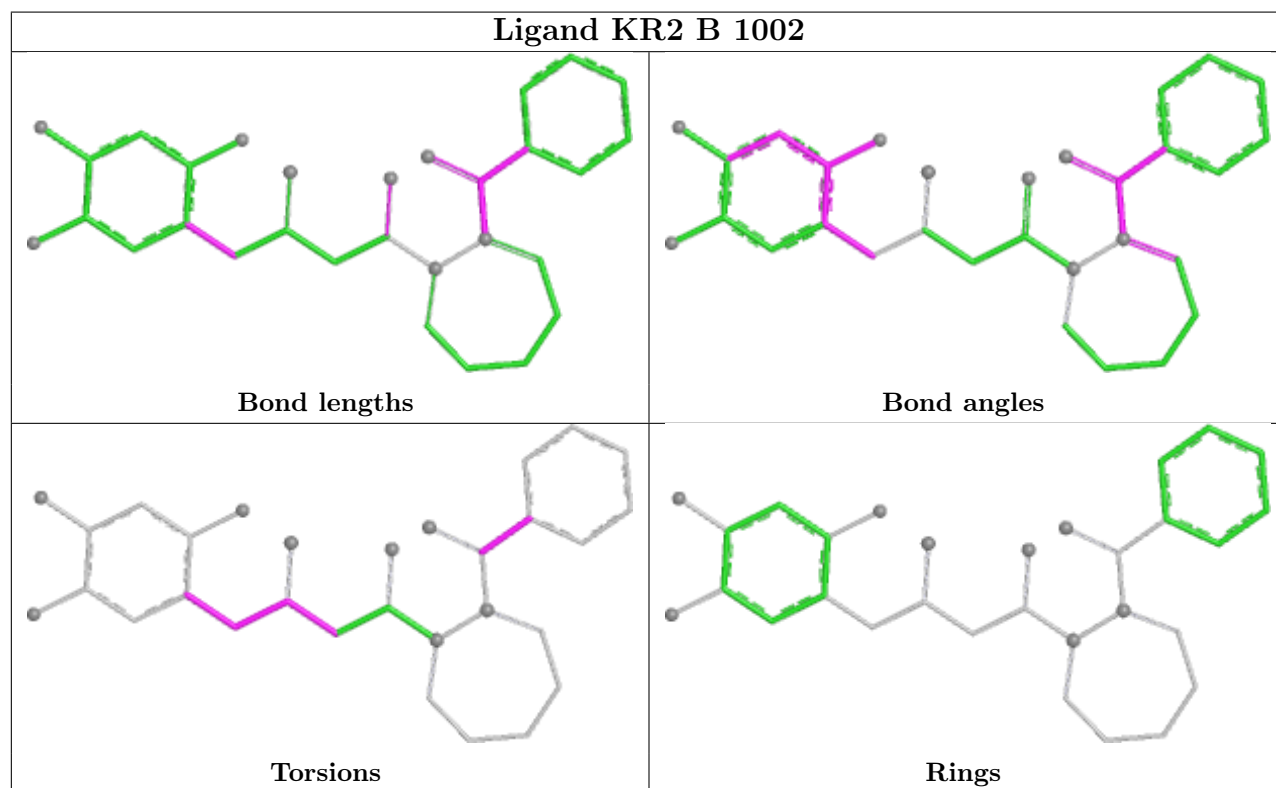
Mol	Chain	Res	Type	Atoms
2	A	1001	KR2	CAF-CAG-CAK-CAL
2	B	1002	KR2	CAF-CAG-CAK-CAL
2	A	1001	KR2	CAH-CAG-CAK-CAL
2	A	1001	KR2	CAG-CAK-CAL-NAM
2	B	1002	KR2	CAH-CAG-CAK-CAL
2	B	1002	KR2	NAR-CAW-CAX-CAZ
2	B	1002	KR2	CAG-CAK-CAL-NAM
2	A	1001	KR2	NAR-CAW-CAX-CAY
2	B	1002	KR2	NAR-CAW-CAX-CAY
2	A	1001	KR2	NAM-CAL-CAN-CAO
2	B	1002	KR2	NAM-CAL-CAN-CAO
2	A	1001	KR2	NAR-CAW-CAX-CAZ
2	B	1002	KR2	CAK-CAL-CAN-CAO

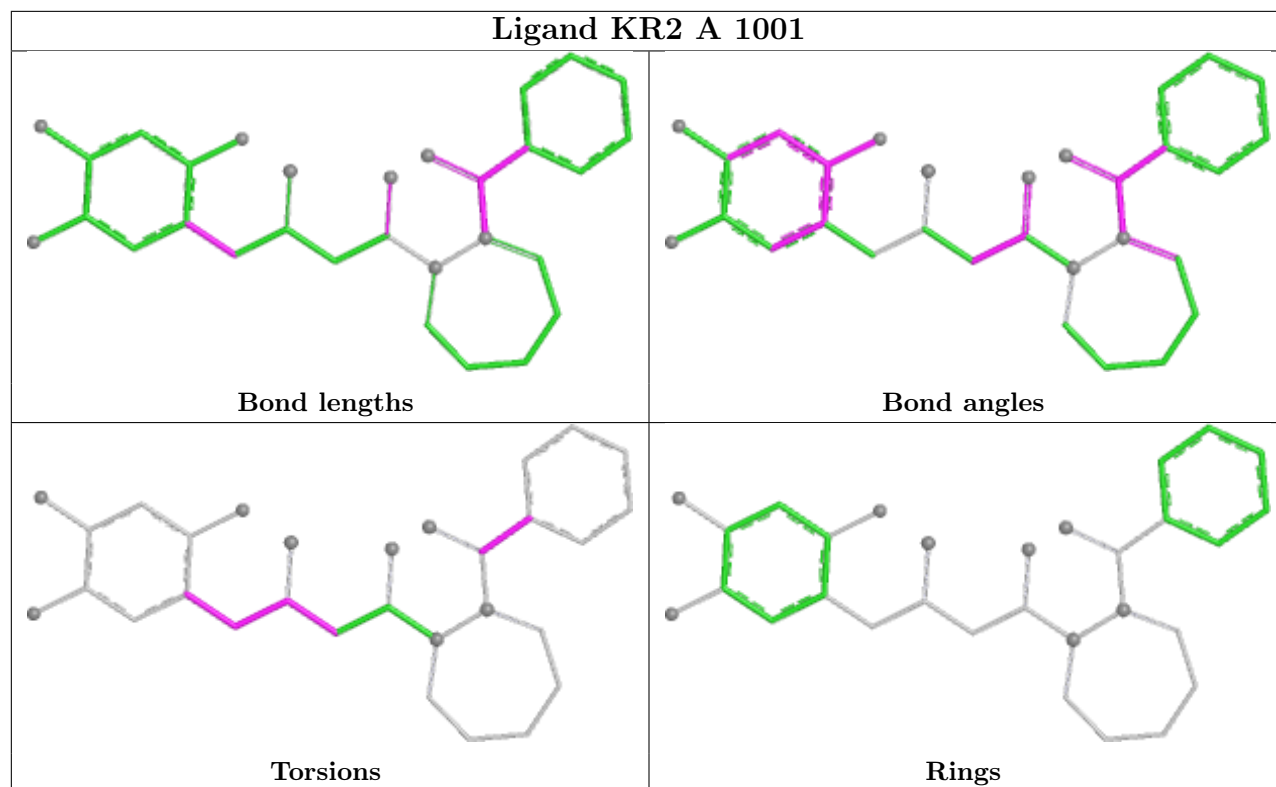
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	KR2	5	0
2	A	1001	KR2	6	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	726/728 (99%)	-0.07	25 (3%)	48 44	14, 27, 59, 94	0
1	B	728/728 (100%)	-0.10	25 (3%)	48 44	11, 26, 61, 93	0
All	All	1454/1456 (99%)	-0.08	50 (3%)	48 44	11, 27, 61, 94	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	5.4
1	B	39	SER	5.4
1	B	390	ASP	5.3
1	B	105	TYR	4.7
1	B	40	ARG	4.5
1	B	277	SER	4.5
1	A	39	SER	4.4
1	B	278	SER	4.4
1	A	40	ARG	4.3
1	A	277	SER	4.1
1	A	105	TYR	4.0
1	A	278	SER	3.7
1	B	366	LEU	3.6
1	B	279	VAL	3.6
1	A	72	GLN	3.5
1	B	506	ASN	3.5
1	B	765	LEU	3.5
1	B	766	PRO	3.4
1	A	392	LYS	3.2
1	A	98	PHE	3.1
1	B	389	ILE	3.1
1	A	73	GLU	3.1
1	A	487	ASN	3.0
1	B	392	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	74	ASN	2.6
1	A	280	THR	2.6
1	B	388	GLN	2.6
1	A	76	ILE	2.5
1	A	74	ASN	2.5
1	B	41	LYS	2.4
1	A	95	PHE	2.3
1	A	66	HIS	2.3
1	B	92	ASN	2.3
1	A	521	GLU	2.3
1	A	88	VAL	2.3
1	B	98	PHE	2.2
1	A	276	LEU	2.2
1	B	343	ARG	2.2
1	B	280	THR	2.2
1	A	77	LEU	2.2
1	B	110	ASP	2.2
1	B	275	SER	2.2
1	B	83	TYR	2.1
1	A	379	GLU	2.1
1	B	393	ASP	2.1
1	A	99	GLY	2.1
1	B	391	LYS	2.1
1	A	93	SER	2.1
1	A	441	LYS	2.0
1	A	538	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

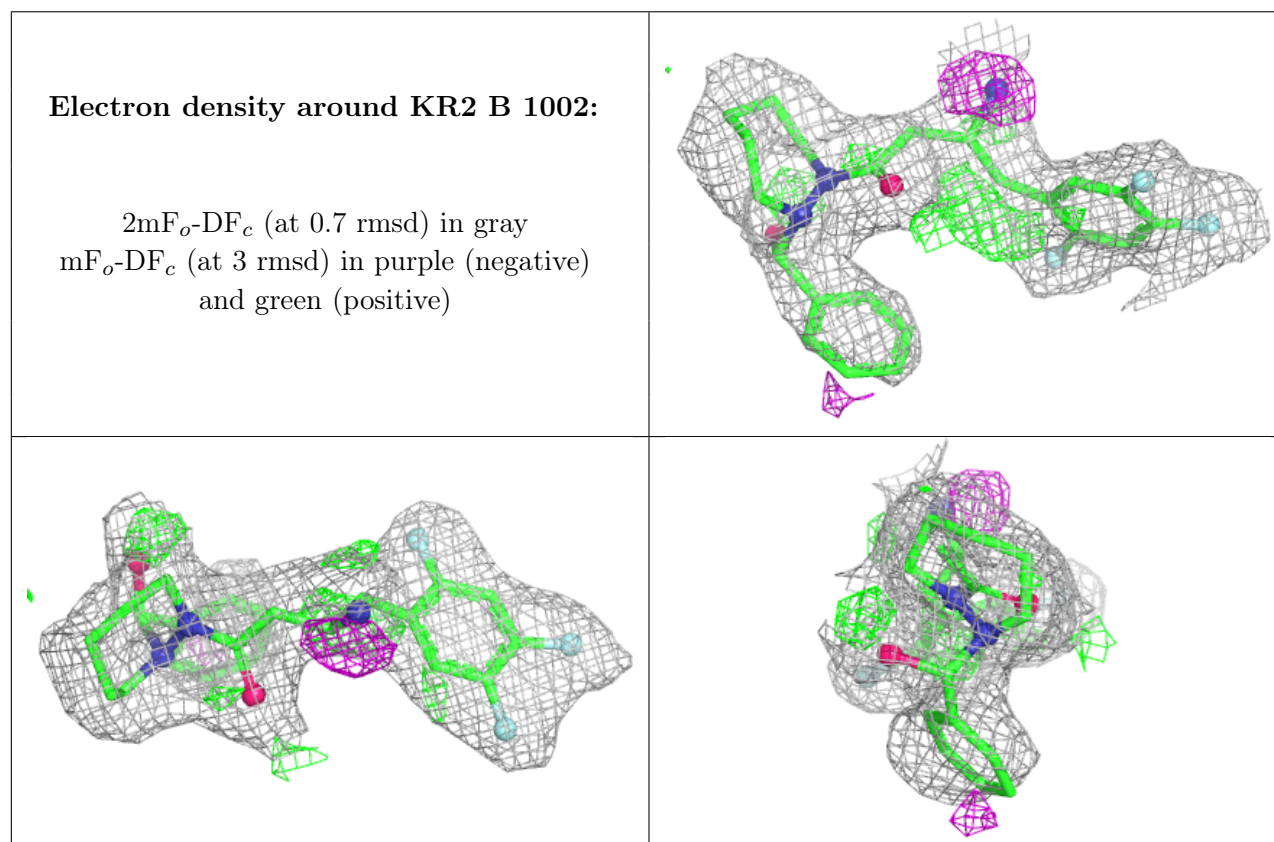
There are no oligosaccharides in this entry.

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.

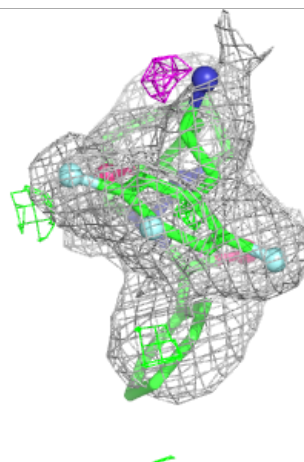
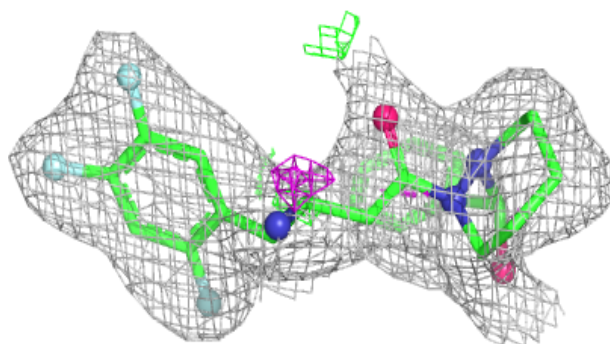
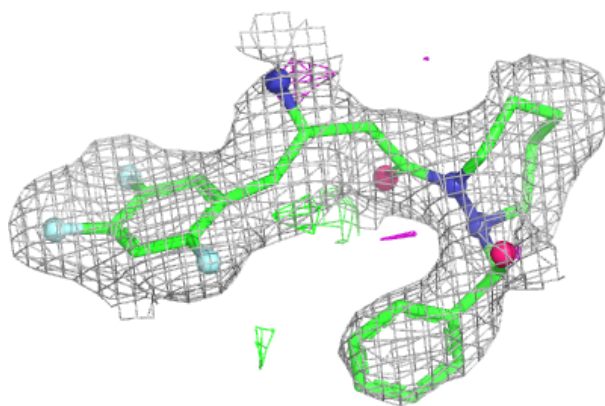
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KR2	B	1002	30/30	0.87	0.15	24,40,64,67	0
2	KR2	A	1001	30/30	0.88	0.12	24,34,61,63	0

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 KR2 A 1001:

$2mF_o-DF_c$ (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.