



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 2V22 / pdb_00002v22
Title : REPLACE: A strategy for Iterative Design of Cyclin Binding Groove Inhibitors
Authors : Andrews, M.J.; Kontopidis, G.; McInnes, C.; Plater, A.; Innes, L.; Cowan, A.;
Jewsbury, P.; Fischer, P.M.
Deposited on : 2007-05-31
Resolution : 2.60 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

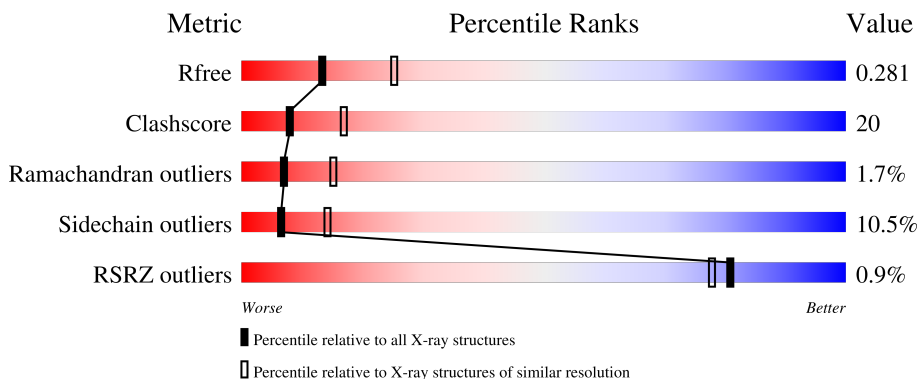
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	298	0.5% 57% 34% 7% 0.5%
1	C	298	2% 67% 21% 10% 0.5%
2	B	259	0.5% 67% 28% 5%
2	D	259	61% 32% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9357 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.

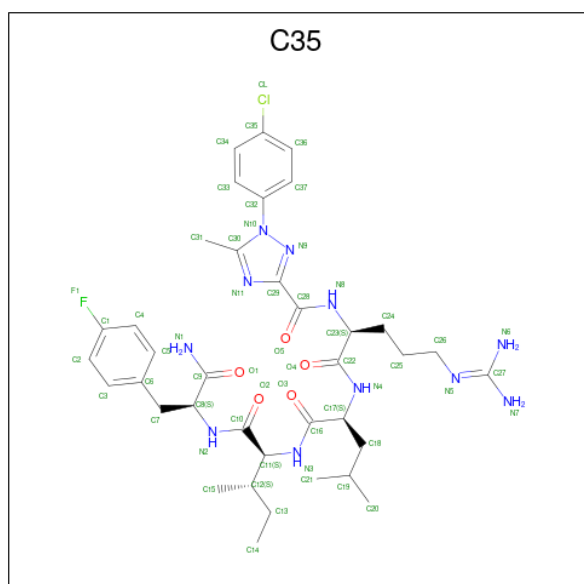
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	297	Total	C	N	O	S	0	0	1
			2379	1547	404	420	8			

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is N 2 -{[1-(4-CHLOROPHENYL)-5-METHYL-1H-1,2,4-TRIAZOL-3-YL]CARBONYL}-N 5 -(DIAMINOMETHYLIDENE)-L-ORNITHYL-L-LEUCYL-L-ISOLEUCYL-4-FLUORO-L-PHENYLALANINAMIDE (CCD ID: C35) (formula: $C_{37}H_{51}ClFN_{11}O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			55	37	1	1	11	5		
3	D	1	Total	C	Cl	F	N	O	0	0
			55	37	1	1	11	5		

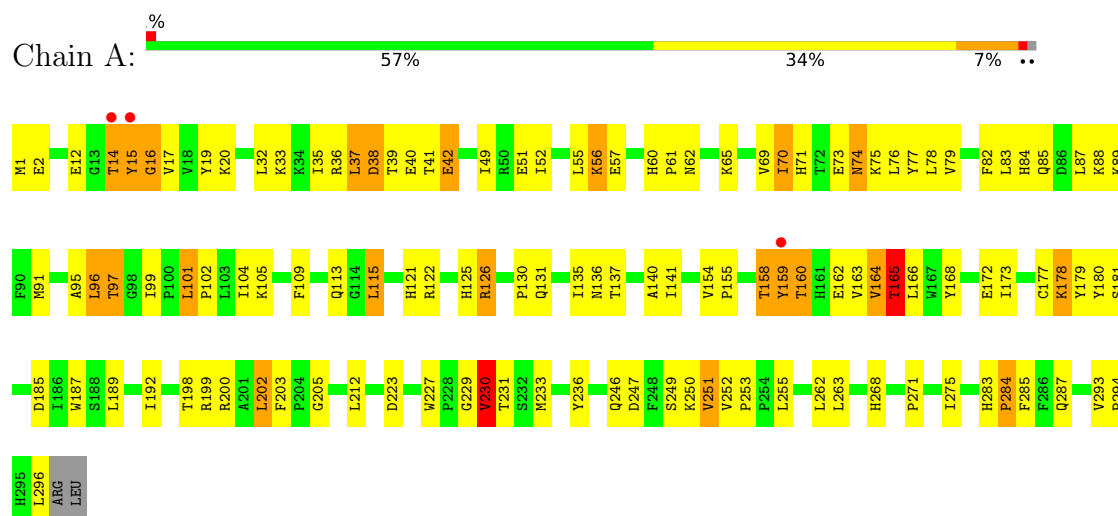
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	83	Total	O	0	0
			83	83		
4	C	76	Total	O	0	0
			76	76		
4	D	94	Total	O	0	0
			94	94		

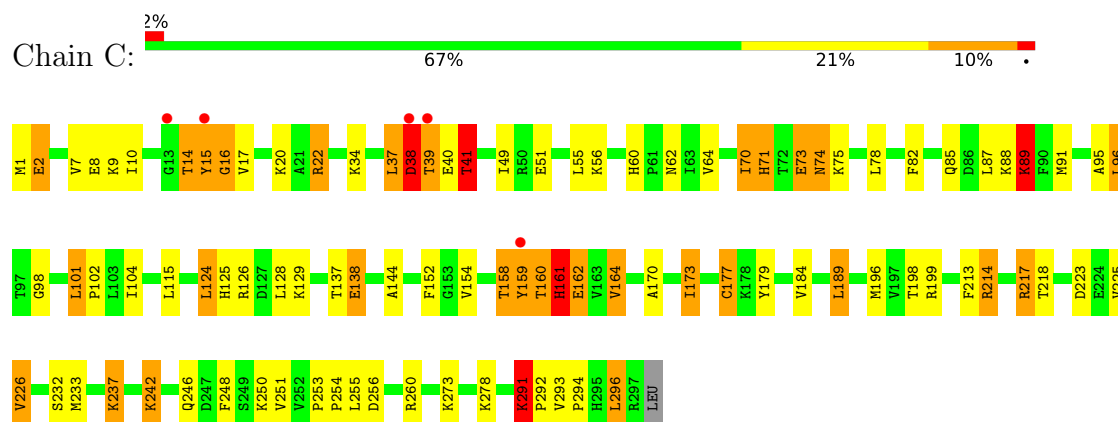
3 Residue-property plots

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.

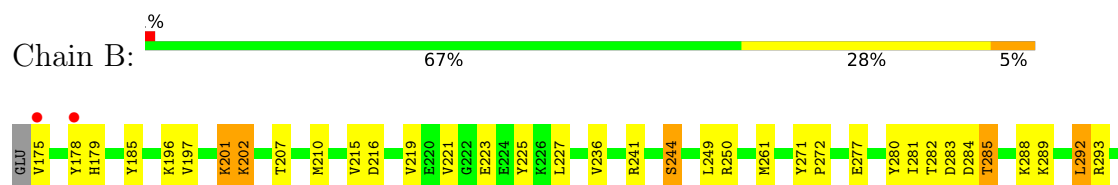
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 1: CELL DIVISION PROTEIN KINASE 2

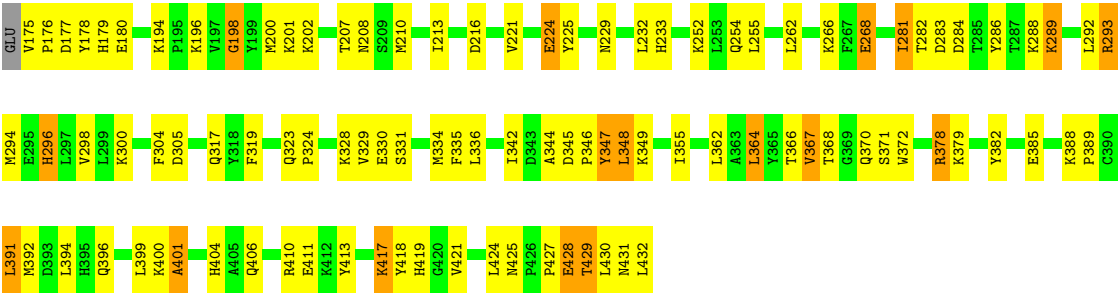


• Molecule 2: CYCLIN-A2





● Molecule 2: CYCLIN-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.69Å 113.57Å 156.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 2.60 16.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (16.00-2.60) 94.4 (16.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.277 0.177 , 0.281	Depositor DCC
R_{free} test set	1235 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: C35

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	0.60	0/2440	1.08	7/3313 (0.2%)
1	C	0.62	1/2441 (0.0%)	1.20	22/3315 (0.7%)
2	B	0.59	0/2133	1.16	14/2896 (0.5%)
2	D	0.61	0/2134	1.16	12/2897 (0.4%)
All	All	0.60	1/9148 (0.0%)	1.15	55/12421 (0.4%)

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	C	0	2
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	LYS	CD-CE	5.09	1.67	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	TYR	N-CA-C	9.38	123.98	112.54
1	C	233	MET	CA-C-N	8.75	128.34	119.24
1	C	233	MET	C-N-CA	8.75	128.34	119.24
1	C	179	TYR	N-CA-C	8.02	122.17	109.50
2	B	372	TRP	CA-C-N	8.01	127.96	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	TRP	C-N-CA	8.01	127.96	120.03
2	D	342	ILE	N-CA-C	7.32	118.11	110.72
2	D	401	ALA	CA-C-N	-6.77	112.83	119.87
2	D	401	ALA	C-N-CA	-6.77	112.83	119.87
1	C	144	ALA	N-CA-C	6.58	117.82	108.74
1	C	291	LYS	CA-C-N	6.55	126.52	119.78
1	C	291	LYS	C-N-CA	6.55	126.52	119.78
1	C	177	CYS	N-CA-C	6.41	119.32	110.35
2	B	215	VAL	N-CA-C	6.31	117.05	110.62
1	A	192	ILE	N-CA-C	-6.30	104.13	111.00
1	C	73	GLU	N-CA-C	5.93	118.70	111.82
1	A	85	GLN	N-CA-C	5.92	116.22	107.88
1	C	14	THR	N-CA-C	5.90	117.82	110.91
2	B	381	GLY	N-CA-C	-5.89	104.70	114.48
2	D	370	GLN	N-CA-C	5.82	118.87	109.79
1	A	69	VAL	CB-CA-C	-5.70	102.68	110.77
1	C	173	ILE	N-CA-C	5.69	115.88	110.42
2	D	268	GLU	N-CA-C	5.69	120.35	113.41
1	C	273	LYS	N-CA-C	-5.68	106.34	113.72
1	C	125	HIS	N-CA-C	5.64	117.10	111.07
1	C	225	VAL	N-CA-C	5.60	115.69	110.42
1	A	251	VAL	N-CA-C	5.56	115.76	110.42
2	D	419	HIS	N-CA-C	-5.54	106.10	112.86
2	B	301	VAL	N-CA-C	5.51	116.24	110.62
2	D	355	ILE	N-CA-C	5.47	116.10	110.36
1	C	64	VAL	CB-CA-C	-5.43	102.38	111.29
2	B	292	LEU	N-CA-C	5.39	117.16	111.28
1	A	230	VAL	CB-CA-C	-5.39	104.98	112.04
2	B	332	LEU	N-CA-C	-5.39	105.49	111.36
2	B	390	CYS	N-CA-C	5.38	116.83	111.07
2	D	213	ILE	N-CA-C	-5.38	105.29	110.72
1	A	271	PRO	N-CA-C	-5.22	106.60	113.65
1	C	251	VAL	CB-CA-C	-5.20	105.28	112.24
2	B	401	ALA	CA-C-N	-5.19	114.73	119.82
2	B	401	ALA	C-N-CA	-5.19	114.73	119.82
1	C	293	VAL	CA-C-N	-5.18	114.65	120.14
1	C	293	VAL	C-N-CA	-5.18	114.65	120.14
2	B	236	VAL	N-CA-C	5.18	115.39	110.42
1	C	129	LYS	CA-C-N	5.16	125.20	119.32
1	C	129	LYS	C-N-CA	5.16	125.20	119.32
2	D	367	VAL	N-CA-C	5.15	116.56	111.67
2	D	194	LYS	CA-C-N	5.14	125.07	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	194	LYS	C-N-CA	5.14	125.07	119.78
2	D	347	TYR	N-CA-C	5.13	119.39	113.18
1	C	89	LYS	N-CA-C	-5.12	105.88	111.82
2	B	244	SER	N-CA-C	5.09	116.83	111.28
1	C	237	LYS	CA-C-N	-5.05	114.84	120.45
1	C	237	LYS	C-N-CA	-5.05	114.84	120.45
2	B	280	TYR	N-CA-C	5.02	117.41	111.33
1	A	168	TYR	N-CA-C	-5.01	104.98	112.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ILE	Peptide
1	C	161	HIS	Peptide
1	C	70	ILE	Peptide
2	D	198	GLY	Peptide

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	2378	0	2426	117	1
1	C	2379	0	2426	104	0
2	B	2083	0	2107	68	0
2	D	2084	0	2107	84	0
3	B	55	0	51	4	1
3	D	55	0	51	1	0
4	A	70	0	0	5	0
4	B	83	0	0	12	0
4	C	76	0	0	7	0
4	D	94	0	0	13	0
All	All	9357	0	9168	356	1

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 (356) 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:16:GLY:HA2	4:A:2008:HOH:O	1.39	1.21
2:B:282:THR:HB	2:B:285:THR:CG2	1.73	1.18
1:C:22:ARG:HG3	1:C:22:ARG:HH11	0.91	1.07
2:B:404:HIS:CD2	2:B:406:GLN:H	1.73	1.05
1:C:214:ARG:HH11	1:C:214:ARG:CG	1.72	1.02
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.36	1.00
1:C:60:HIS:HD2	1:C:62:ASN:H	1.07	0.99
1:A:1:MET:HE2	1:A:70:ILE:HD12	1.45	0.98
1:C:159:TYR:O	1:C:161:HIS:N	1.97	0.98
1:C:22:ARG:HG3	1:C:22:ARG:NH1	1.61	0.97
2:B:379:LYS:HE2	4:B:2041:HOH:O	1.65	0.96
1:C:214:ARG:HH11	1:C:214:ARG:HG3	1.29	0.95
2:D:207:THR:HG22	2:D:210:MET:HG3	1.48	0.95
2:B:321:HIS:CE1	2:B:379:LYS:HD3	2.01	0.94
1:A:14:THR:O	1:A:15:TYR:CD1	2.20	0.93
2:B:282:THR:O	2:B:285:THR:HG22	1.66	0.93
2:B:404:HIS:HD2	2:B:406:GLN:N	1.65	0.93
1:C:60:HIS:CD2	1:C:62:ASN:H	1.86	0.92
2:D:404:HIS:HD2	2:D:406:GLN:H	0.97	0.92
1:C:22:ARG:HH11	1:C:22:ARG:CG	1.78	0.91
2:B:282:THR:HB	2:B:285:THR:HG23	1.50	0.90
1:C:162:GLU:OE1	1:C:164:VAL:HG23	1.69	0.90
1:A:71:HIS:CE1	2:B:296:HIS:CE1	2.61	0.89
1:A:60:HIS:HD2	1:A:62:ASN:H	1.18	0.89
2:B:304:PHE:HD1	4:B:2037:HOH:O	1.55	0.89
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.53	0.89
2:D:224:GLU:HG3	4:D:2022:HOH:O	1.72	0.89
2:B:282:THR:O	2:B:285:THR:CG2	2.23	0.87
2:D:378:ARG:CB	2:D:378:ARG:HH11	1.88	0.87
2:D:417:LYS:HD2	2:D:418:TYR:CE2	2.09	0.87
1:A:162:GLU:HG3	1:A:164:VAL:HB	1.56	0.86
1:C:173:ILE:HD11	1:C:184:VAL:CG1	2.05	0.86
2:D:404:HIS:CD2	2:D:406:GLN:H	1.90	0.86
1:C:162:GLU:OE1	1:C:164:VAL:CG2	2.24	0.85
2:B:282:THR:CB	2:B:285:THR:CG2	2.55	0.85
2:B:207:THR:HG23	2:B:210:MET:H	1.40	0.85
1:C:95:ALA:O	1:C:96:LEU:HB3	1.77	0.85
2:D:300:LYS:HE2	4:D:2047:HOH:O	1.76	0.84
2:D:379:LYS:HE3	4:D:2008:HOH:O	1.78	0.84
1:A:95:ALA:O	1:A:96:LEU:HB3	1.78	0.84
1:A:84:HIS:CE1	1:A:296:LEU:HG	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASP:O	1:C:40:GLU:N	2.10	0.83
1:A:60:HIS:CD2	1:A:62:ASN:H	1.97	0.82
1:C:96:LEU:H	1:C:199:ARG:HH11	1.23	0.82
1:C:278:LYS:NZ	2:D:177:ASP:O	2.11	0.82
1:A:231:THR:HG22	1:A:236:TYR:CE1	2.14	0.82
1:C:161:HIS:N	1:C:161:HIS:CD2	2.47	0.81
2:D:378:ARG:HH11	2:D:378:ARG:CG	1.93	0.81
2:B:282:THR:HB	2:B:285:THR:HG21	1.61	0.81
2:D:417:LYS:HE2	4:D:2001:HOH:O	1.81	0.81
1:C:51:GLU:O	1:C:55:LEU:HB2	1.81	0.81
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.65	0.78
1:C:1:MET:HE2	1:C:70:ILE:HD12	1.64	0.78
1:A:17:VAL:HG13	1:A:19:TYR:HE1	1.47	0.78
2:D:221:VAL:HG22	2:D:281:ILE:HD13	1.64	0.78
2:B:207:THR:HG22	2:B:210:MET:HG3	1.65	0.76
1:A:38:ASP:OD2	1:A:41:THR:HB	1.84	0.75
1:C:198:THR:O	1:C:199:ARG:HB2	1.85	0.75
1:C:177:CYS:SG	4:C:2008:HOH:O	2.45	0.75
1:A:162:GLU:CG	1:A:164:VAL:HB	2.15	0.75
1:C:214:ARG:HG3	1:C:214:ARG:NH1	1.99	0.75
1:A:159:TYR:HD1	1:A:159:TYR:N	1.87	0.73
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.70	0.71
2:D:418:TYR:O	2:D:421:VAL:HG13	1.91	0.71
1:C:60:HIS:HD2	1:C:62:ASN:N	1.84	0.71
1:A:164:VAL:HG12	1:A:164:VAL:O	1.91	0.69
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.75	0.69
1:C:96:LEU:H	1:C:199:ARG:NH1	1.89	0.69
1:A:17:VAL:HG13	1:A:19:TYR:CE1	2.27	0.69
1:C:159:TYR:HB3	1:C:162:GLU:HB3	1.74	0.69
1:A:231:THR:HA	1:A:236:TYR:CD1	2.29	0.68
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.12	0.68
1:A:172:GLU:HG2	1:A:173:ILE:HD12	1.74	0.68
1:C:177:CYS:SG	4:C:2020:HOH:O	2.51	0.68
1:A:1:MET:CE	1:A:70:ILE:HD12	2.23	0.67
1:A:84:HIS:HE1	1:A:296:LEU:HG	1.58	0.67
2:D:392:MET:HE2	2:D:392:MET:HA	1.77	0.67
1:C:160:THR:C	1:C:161:HIS:CD2	2.73	0.66
2:B:216:ASP:OD1	2:B:408:SER:HB2	1.95	0.66
1:A:159:TYR:N	1:A:159:TYR:CD1	2.60	0.66
1:C:159:TYR:HB2	1:C:162:GLU:HG2	1.78	0.66
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:GLN:O	2:D:323:GLN:HG2	1.95	0.66
1:A:165:THR:N	4:A:2049:HOH:O	2.27	0.66
2:B:321:HIS:HE1	2:B:379:LYS:HD3	1.57	0.66
1:C:1:MET:CE	1:C:70:ILE:HD12	2.25	0.66
1:C:137:THR:HG22	1:C:296:LEU:HD23	1.77	0.66
1:A:96:LEU:HD23	1:A:97:THR:HG22	1.79	0.65
2:B:282:THR:C	2:B:285:THR:HG22	2.21	0.65
2:B:201:LYS:HD3	4:B:2007:HOH:O	1.97	0.65
1:C:161:HIS:N	1:C:161:HIS:HD2	1.92	0.65
1:C:40:GLU:O	2:D:288:LYS:HE2	1.96	0.65
1:C:15:TYR:HA	4:C:2005:HOH:O	1.97	0.65
1:A:40:GLU:HB2	4:B:2029:HOH:O	1.97	0.65
1:C:7:VAL:HG12	1:C:8:GLU:HG2	1.78	0.65
2:B:282:THR:CB	2:B:285:THR:HG23	2.23	0.65
2:B:207:THR:HG21	4:B:2012:HOH:O	1.98	0.64
1:A:227:TRP:O	1:A:230:VAL:HG22	1.98	0.64
1:A:198:THR:O	1:A:199:ARG:HB2	1.96	0.64
2:D:323:GLN:HB2	4:D:2058:HOH:O	1.96	0.64
1:C:214:ARG:HH11	1:C:214:ARG:HG2	1.58	0.64
2:D:378:ARG:NH1	2:D:378:ARG:HG2	2.12	0.63
1:A:84:HIS:HB2	4:A:2033:HOH:O	1.99	0.63
2:B:216:ASP:CG	2:B:408:SER:HB2	2.23	0.63
2:D:268:GLU:HG3	2:D:268:GLU:O	1.99	0.62
1:C:159:TYR:CB	1:C:162:GLU:HG2	2.29	0.62
1:A:36:ARG:O	1:A:36:ARG:HG2	1.99	0.62
2:D:202:LYS:HE2	4:D:2015:HOH:O	1.99	0.62
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.29	0.62
2:D:175:VAL:O	2:D:175:VAL:HG13	2.00	0.61
2:D:378:ARG:CG	2:D:378:ARG:NH1	2.56	0.61
2:B:388:LYS:O	2:B:392:MET:HG3	2.01	0.61
1:C:22:ARG:NH1	1:C:22:ARG:CG	2.43	0.61
1:C:159:TYR:HB3	1:C:162:GLU:CB	2.29	0.61
2:B:207:THR:CG2	2:B:210:MET:HG3	2.31	0.61
2:B:241:ARG:O	2:B:244:SER:HB2	2.01	0.61
2:B:430:LEU:O	2:B:431:ASN:HB2	2.01	0.61
2:D:207:THR:HG23	2:D:210:MET:H	1.66	0.60
1:A:14:THR:O	1:A:15:TYR:HD1	1.77	0.60
1:A:121:HIS:C	1:A:122:ARG:HG3	2.26	0.60
1:C:218:THR:HA	1:C:246:GLN:HE21	1.66	0.60
2:B:304:PHE:CD1	4:B:2037:HOH:O	2.40	0.60
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.84	0.60
1:A:121:HIS:O	1:A:122:ARG:HG3	2.02	0.60
2:D:404:HIS:HD2	2:D:406:GLN:N	1.83	0.59
1:A:227:TRP:O	1:A:230:VAL:CG2	2.49	0.59
1:C:294:PRO:HB2	1:C:296:LEU:HD13	1.84	0.59
1:C:16:GLY:HA3	1:C:34:LYS:O	2.02	0.59
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.84	0.59
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.43	0.59
2:B:403:GLN:HG2	4:B:2064:HOH:O	2.03	0.59
2:D:283:ASP:HB2	3:D:1433:C35:N11	2.18	0.58
2:B:396:GLN:HG3	4:B:2062:HOH:O	2.02	0.58
2:B:207:THR:CG2	2:B:210:MET:H	2.12	0.58
1:C:37:LEU:O	1:C:39:THR:N	2.37	0.58
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.29	0.58
2:D:207:THR:CG2	2:D:210:MET:HG3	2.26	0.58
1:C:73:GLU:CD	2:D:293:ARG:NH2	2.62	0.58
1:A:14:THR:C	1:A:15:TYR:CD1	2.82	0.57
1:A:14:THR:C	1:A:15:TYR:HD1	2.12	0.57
2:B:293:ARG:HD2	4:B:2032:HOH:O	2.04	0.57
1:C:124:LEU:HD12	1:C:126:ARG:HG2	1.86	0.57
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.86	0.57
2:B:345:ASP:HB2	2:B:346:PRO:HD3	1.87	0.57
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.40	0.57
2:D:378:ARG:HH11	2:D:378:ARG:HB2	1.68	0.57
1:C:115:LEU:CD1	1:C:189:LEU:HD22	2.34	0.57
2:B:421:VAL:O	2:B:424:LEU:HB2	2.04	0.57
1:C:115:LEU:HD12	1:C:189:LEU:CD2	2.34	0.56
2:B:207:THR:HG22	2:B:210:MET:CG	2.34	0.56
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.88	0.56
2:B:282:THR:O	2:B:285:THR:HG21	2.06	0.56
1:C:98:GLY:CA	1:C:199:ARG:HD3	2.33	0.56
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.87	0.56
1:A:96:LEU:CD2	1:A:97:THR:HG22	2.36	0.55
2:D:323:GLN:HG3	4:D:2057:HOH:O	2.06	0.55
1:C:1:MET:N	4:C:2001:HOH:O	2.38	0.55
1:C:96:LEU:N	1:C:199:ARG:NH1	2.54	0.55
2:D:378:ARG:HH11	2:D:378:ARG:HG2	1.68	0.55
2:B:319:PHE:CE2	2:B:330:GLU:HG2	2.42	0.55
1:C:260:ARG:NH1	4:C:2069:HOH:O	2.38	0.55
2:D:282:THR:O	2:D:283:ASP:CB	2.54	0.55
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:CE1	2:D:296:HIS:CE1	2.96	0.54
1:C:159:TYR:C	1:C:161:HIS:N	2.65	0.54
1:C:173:ILE:CD1	1:C:184:VAL:CG1	2.83	0.54
1:A:16:GLY:H	1:A:36:ARG:NH2	2.06	0.54
1:A:121:HIS:CD2	2:B:185:TYR:CE1	2.95	0.54
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.38	0.54
2:D:346:PRO:O	2:D:349:LYS:HG3	2.07	0.54
2:B:389:PRO:HB3	4:B:2051:HOH:O	2.06	0.54
1:A:125:HIS:O	1:A:126:ARG:HB2	2.08	0.54
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.43	0.53
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.90	0.53
3:B:1433:C35:H33	3:B:1433:C35:C31	2.38	0.53
1:C:9:LYS:HE3	4:C:2004:HOH:O	2.09	0.53
2:D:282:THR:O	2:D:283:ASP:HB3	2.08	0.53
1:C:170:ALA:HB3	1:C:173:ILE:HD12	1.91	0.53
1:A:51:GLU:O	1:A:55:LEU:HB2	2.09	0.53
2:D:385:GLU:HB2	4:D:2068:HOH:O	2.08	0.53
1:C:40:GLU:O	2:D:288:LYS:CE	2.57	0.53
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.73	0.53
1:A:36:ARG:O	1:A:36:ARG:CG	2.57	0.52
1:A:247:ASP:HB3	1:A:250:LYS:HD2	1.91	0.52
1:C:22:ARG:HD2	4:C:2007:HOH:O	2.08	0.52
1:C:291:LYS:N	1:C:292:PRO:CD	2.73	0.52
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.39	0.52
3:B:1433:C35:C31	3:B:1433:C35:C33	2.86	0.52
1:C:2:GLU:H	1:C:2:GLU:CD	2.18	0.52
1:C:60:HIS:CD2	1:C:62:ASN:N	2.67	0.52
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.24	0.52
2:D:207:THR:HG22	2:D:210:MET:CG	2.30	0.52
1:A:162:GLU:HG3	1:A:164:VAL:CB	2.33	0.52
2:D:430:LEU:O	2:D:431:ASN:HB2	2.10	0.52
1:A:178:LYS:HE2	1:A:179:TYR:CE2	2.46	0.51
1:A:294:PRO:HG2	1:A:296:LEU:HD22	1.92	0.51
2:B:283:ASP:HB2	3:B:1433:C35:N11	2.26	0.51
1:A:60:HIS:HD2	1:A:62:ASN:N	2.00	0.51
1:C:160:THR:HA	1:C:161:HIS:CD2	2.45	0.51
1:A:20:LYS:HE2	1:A:82:PHE:CZ	2.45	0.51
1:A:158:THR:OG1	1:A:178:LYS:HA	2.10	0.51
2:D:428:GLU:C	2:D:429:THR:CG2	2.83	0.51
2:D:428:GLU:O	2:D:429:THR:HG22	2.10	0.51
1:A:96:LEU:HD23	1:A:96:LEU:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:HE2	1:A:35:ILE:CD1	2.24	0.50
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.45	0.50
2:B:404:HIS:HD2	2:B:406:GLN:H	0.81	0.50
1:C:91:MET:CE	1:C:196:MET:HG3	2.41	0.50
1:A:135:ILE:CG2	1:A:141:ILE:HG13	2.41	0.50
1:A:162:GLU:OE1	1:A:180:TYR:OH	2.26	0.50
1:A:38:ASP:C	1:A:38:ASP:OD1	2.55	0.50
2:D:221:VAL:HG22	2:D:281:ILE:CD1	2.37	0.50
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.94	0.50
1:A:42:GLU:OE2	1:A:42:GLU:HA	2.12	0.50
2:D:396:GLN:HE21	2:D:396:GLN:HA	1.76	0.50
1:A:251:VAL:HG12	1:A:252:VAL:HG13	1.93	0.49
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.40	0.49
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.94	0.49
1:A:15:TYR:CD2	1:A:35:ILE:HG12	2.47	0.49
2:D:347:TYR:OH	2:D:394:LEU:HA	2.12	0.49
1:A:52:ILE:O	1:A:56:LYS:HB2	2.12	0.49
1:C:74:ASN:N	1:C:74:ASN:OD1	2.45	0.49
1:C:20:LYS:HD2	1:C:82:PHE:CZ	2.48	0.49
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.94	0.49
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.94	0.49
1:C:124:LEU:HD12	1:C:126:ARG:CG	2.43	0.49
1:A:229:GLY:O	1:A:230:VAL:C	2.55	0.49
2:D:255:LEU:HB2	2:D:286:TYR:CZ	2.48	0.49
1:A:135:ILE:HG22	1:A:141:ILE:HG13	1.95	0.48
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.13	0.48
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.94	0.48
1:A:16:GLY:H	1:A:36:ARG:HH21	1.60	0.48
1:C:223:ASP:OD1	1:C:226:VAL:HG23	2.14	0.48
1:C:124:LEU:HD23	1:C:152:PHE:CD1	2.48	0.48
1:A:159:TYR:O	1:A:160:THR:C	2.57	0.48
1:A:154:VAL:HG13	1:A:155:PRO:HD2	1.96	0.47
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.49	0.47
1:A:173:ILE:HD12	1:A:173:ILE:N	2.29	0.47
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.69	0.47
1:A:87:LEU:O	1:A:91:MET:HG3	2.14	0.47
1:A:137:THR:HG22	1:A:296:LEU:HD23	1.95	0.47
2:D:178:TYR:C	2:D:178:TYR:CD2	2.92	0.47
2:B:277:GLU:HG3	4:B:2028:HOH:O	2.15	0.47
2:D:233:HIS:HD2	4:D:2051:HOH:O	1.98	0.47
1:A:49:ILE:HG23	2:B:306:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:HG21	2:B:409:ILE:HG13	1.97	0.47
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.50	0.47
1:A:74:ASN:H	1:A:74:ASN:ND2	2.13	0.46
1:C:56:LYS:HE2	2:D:305:ASP:OD1	2.16	0.46
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.96	0.46
1:C:159:TYR:CD1	1:C:162:GLU:CD	2.93	0.46
2:D:216:ASP:OD1	2:D:406:GLN:HB3	2.15	0.46
2:D:391:LEU:HD23	2:D:432:LEU:HD11	1.96	0.46
1:A:91:MET:HG2	1:A:99:ILE:CD1	2.45	0.46
2:B:227:LEU:CD1	2:B:261:MET:HE3	2.45	0.46
1:C:71:HIS:ND1	2:D:296:HIS:CE1	2.83	0.46
1:C:96:LEU:N	1:C:199:ARG:HH11	1.99	0.46
2:D:371:SER:O	2:D:372:TRP:C	2.58	0.46
2:D:198:GLY:HA3	4:D:2015:HOH:O	2.15	0.45
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.51	0.45
1:C:255:LEU:O	1:C:260:ARG:NH1	2.48	0.45
2:D:317:GLN:HG2	4:D:2054:HOH:O	2.16	0.45
1:A:101:LEU:CB	1:A:102:PRO:HD3	2.46	0.45
2:B:178:TYR:O	2:B:179:HIS:C	2.60	0.45
1:C:49:ILE:HD12	1:C:49:ILE:HG23	1.72	0.45
1:C:104:ILE:HG23	1:C:196:MET:HE3	1.99	0.45
1:A:199:ARG:HG2	4:A:2034:HOH:O	2.15	0.45
1:C:256:ASP:O	1:C:260:ARG:HG3	2.17	0.45
2:D:294:MET:O	2:D:298:VAL:HG23	2.16	0.45
1:C:101:LEU:N	1:C:102:PRO:CD	2.80	0.45
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.51	0.45
1:A:164:VAL:O	1:A:165:THR:HG22	2.17	0.45
1:C:159:TYR:HB3	1:C:162:GLU:CG	2.47	0.45
1:C:96:LEU:HA	1:C:199:ARG:HH12	1.82	0.44
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.98	0.44
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.33	0.44
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.98	0.44
1:A:37:LEU:HB3	1:A:39:THR:HG23	2.00	0.44
2:B:221:VAL:HG22	2:B:281:ILE:HD13	1.99	0.44
1:A:109:PHE:O	1:A:113:GLN:HG3	2.17	0.44
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.53	0.44
1:A:262:LEU:O	1:A:263:LEU:C	2.59	0.44
2:B:202:LYS:HZ3	2:B:202:LYS:HG2	1.66	0.44
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.83	0.44
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.82	0.44
1:C:160:THR:CA	1:C:161:HIS:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.48	0.43
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.75	0.43
1:A:121:HIS:HD2	2:B:185:TYR:CZ	2.35	0.43
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.85	0.43
2:B:430:LEU:HB3	2:B:432:LEU:HD23	1.99	0.43
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.99	0.43
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.99	0.43
1:C:138:GLU:N	1:C:138:GLU:OE2	2.52	0.43
2:B:289:LYS:HE3	2:B:289:LYS:HB2	1.86	0.43
2:B:336:LEU:HD13	2:B:362:LEU:HD23	2.00	0.43
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.79	0.43
2:B:319:PHE:CD2	2:B:330:GLU:HG2	2.54	0.43
2:D:382:TYR:HE1	4:D:2012:HOH:O	2.02	0.43
1:A:177:CYS:HB2	1:A:233:MET:HE1	1.99	0.43
2:B:322:GLN:NE2	2:B:326:ASN:H	2.17	0.42
2:D:229:ASN:HD22	2:D:334:MET:HE3	1.84	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.89	0.42
1:A:198:THR:CG2	1:A:252:VAL:HG12	2.48	0.42
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.44	0.42
1:C:294:PRO:HG2	1:C:296:LEU:HD13	2.01	0.42
1:A:247:ASP:OD1	1:A:249:SER:HB2	2.19	0.42
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.35	0.42
1:A:70:ILE:HB	1:A:77:TYR:HB2	2.01	0.42
1:C:51:GLU:O	1:C:55:LEU:CB	2.60	0.42
1:A:136:ASN:C	1:A:136:ASN:OD1	2.62	0.42
1:A:253:PRO:O	1:A:255:LEU:N	2.53	0.42
2:B:371:SER:O	2:B:372:TRP:C	2.61	0.42
1:C:73:GLU:OE1	2:D:293:ARG:CZ	2.67	0.42
2:D:289:LYS:HB2	4:D:2044:HOH:O	2.20	0.42
2:D:289:LYS:NZ	2:D:293:ARG:NH1	2.68	0.42
1:A:163:VAL:C	1:A:164:VAL:HG23	2.45	0.42
1:C:189:LEU:HA	1:C:189:LEU:HD12	1.83	0.42
1:A:71:HIS:ND1	2:B:296:HIS:CE1	2.85	0.42
2:D:225:TYR:HE1	2:D:281:ILE:HD12	1.85	0.41
1:C:160:THR:C	1:C:161:HIS:CG	2.99	0.41
1:C:213:PHE:O	1:C:217:ARG:HG2	2.20	0.41
1:A:166:LEU:HD23	1:A:205:GLY:O	2.20	0.41
2:D:252:LYS:HA	2:D:252:LYS:HD2	1.94	0.41
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.55	0.41
1:A:15:TYR:CE2	1:A:35:ILE:HD11	2.56	0.41
2:B:285:THR:HG22	2:B:285:THR:H	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CD2	1:C:62:ASN:HB2	2.56	0.41
1:C:159:TYR:HB3	1:C:162:GLU:HG2	2.03	0.41
2:D:399:LEU:HD23	2:D:399:LEU:HA	1.93	0.41
3:B:1433:C35:H33	3:B:1433:C35:H312	2.03	0.41
1:C:71:HIS:NE2	2:D:304:PHE:CE2	2.87	0.41
1:A:187:TRP:CD1	1:A:187:TRP:C	2.98	0.41
1:C:96:LEU:CA	1:C:199:ARG:NH1	2.84	0.41
1:A:88:LYS:HB2	1:A:130:PRO:HB2	2.02	0.40
2:B:383:THR:O	2:B:384:LEU:C	2.64	0.40
2:D:366:THR:OG1	2:D:427:PRO:HD3	2.21	0.40
1:A:74:ASN:ND2	1:A:74:ASN:N	2.69	0.40
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.56	0.40
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.80	0.40
1:A:101:LEU:O	1:A:104:ILE:HB	2.22	0.40
1:A:105:LYS:HE2	1:A:285:PHE:O	2.22	0.40
1:A:275:ILE:O	1:A:275:ILE:HG23	2.21	0.40
2:D:289:LYS:HZ3	2:D:293:ARG:NH1	2.19	0.40
2:D:331:SER:HB2	2:D:421:VAL:HG11	2.02	0.40
2:D:410:ARG:O	2:D:411:GLU:C	2.63	0.40
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.94	0.40
2:B:339:LEU:HD23	2:B:339:LEU:HA	1.65	0.40
2:B:425:ASN:ND2	4:B:2079:HOH:O	2.55	0.40
1:C:41:THR:O	2:D:288:LYS:HE3	2.22	0.40
1:A:181:SER:OG	4:A:2052:HOH:O	2.22	0.40
1:A:223:ASP:C	1:A:223:ASP:OD1	2.64	0.40
1:A:283:HIS:HA	1:A:284:PRO:HD2	1.86	0.40
1:C:158:THR:HG21	1:C:177:CYS:O	2.20	0.40
2:D:323:GLN:HA	2:D:324:PRO:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:CG2	3:B:1433:C35:C14[4_455]	2.18	0.02

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	294/298 (99%)	263 (90%)	24 (8%)	7 (2%)	4	9
1	C	295/298 (99%)	270 (92%)	18 (6%)	7 (2%)	4	9
2	B	256/259 (99%)	240 (94%)	12 (5%)	4 (2%)	7	16
2	D	256/259 (99%)	242 (94%)	13 (5%)	1 (0%)	30	51
All	All	1101/1114 (99%)	1015 (92%)	67 (6%)	19 (2%)	7	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	160	THR
1	A	15	TYR
2	B	420	GLY
2	D	176	PRO
1	A	38	ASP
1	A	165	THR
2	B	284	ASP
2	B	424	LEU
1	C	15	TYR
1	C	159	TYR
2	B	346	PRO
1	A	16	GLY
1	A	164	VAL
1	C	16	GLY
1	A	284	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	233 (89%)	28 (11%)	6	14
1	C	261/263 (99%)	226 (87%)	35 (13%)	4	7
2	B	232/233 (100%)	214 (92%)	18 (8%)	11	26
2	D	232/233 (100%)	209 (90%)	23 (10%)	7	16
All	All	986/992 (99%)	882 (90%)	104 (10%)	6	14

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	12	GLU
1	A	37	LEU
1	A	42	GLU
1	A	56	LYS
1	A	65	LYS
1	A	74	ASN
1	A	75	LYS
1	A	76	LEU
1	A	89	LYS
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	115	LEU
1	A	126	ARG
1	A	131	GLN
1	A	158	THR
1	A	159	TYR
1	A	160	THR
1	A	165	THR
1	A	178	LYS
1	A	200	ARG
1	A	202	LEU
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	268	HIS
1	A	287	GLN
1	A	293	VAL
2	B	175	VAL
2	B	196	LYS
2	B	197	VAL
2	B	201	LYS
2	B	202	LYS
2	B	249	LEU
2	B	250	ARG
2	B	285	THR
2	B	288	LYS
2	B	292	LEU
2	B	323	GLN
2	B	348	LEU
2	B	400	LYS
2	B	403	GLN
2	B	408	SER
2	B	416	SER
2	B	425	ASN
2	B	432	LEU
1	C	2	GLU
1	C	10	ILE
1	C	14	THR
1	C	17	VAL
1	C	22	ARG
1	C	37	LEU
1	C	38	ASP
1	C	41	THR
1	C	71	HIS
1	C	74	ASN
1	C	75	LYS
1	C	78	LEU
1	C	87	LEU
1	C	88	LYS
1	C	89	LYS
1	C	96	LEU
1	C	101	LEU
1	C	124	LEU
1	C	138	GLU
1	C	154	VAL

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Mol	Chain	Res	Type
1	C	158	THR
1	C	161	HIS
1	C	162	GLU
1	C	164	VAL
1	C	189	LEU
1	C	214	ARG
1	C	217	ARG
1	C	226	VAL
1	C	232	SER
1	C	237	LYS
1	C	242	LYS
1	C	248	PHE
1	C	250	LYS
1	C	291	LYS
1	C	296	LEU
2	D	179	HIS
2	D	180	GLU
2	D	196	LYS
2	D	201	LYS
2	D	224	GLU
2	D	232	LEU
2	D	281	ILE
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU
2	D	293	ARG
2	D	296	HIS
2	D	328	LYS
2	D	348	LEU
2	D	364	LEU
2	D	378	ARG
2	D	391	LEU
2	D	400	LYS
2	D	417	LYS
2	D	424	LEU
2	D	425	ASN
2	D	428	GLU
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	113	GLN
1	A	121	HIS
1	A	131	GLN
1	A	246	GLN
2	B	208	ASN
2	B	296	HIS
2	B	312	ASN
2	B	322	GLN
2	B	323	GLN
2	B	404	HIS
2	B	431	ASN
1	C	60	HIS
1	C	85	GLN
1	C	131	GLN
1	C	161	HIS
1	C	287	GLN
2	D	183	HIS
2	D	208	ASN
2	D	296	HIS
2	D	322	GLN
2	D	396	GLN
2	D	403	GLN
2	D	404	HIS
2	D	419	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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
3	C35	B	1433	-	57,57,57	1.63	6 (10%)	71,78,78	1.52	12 (16%)
3	C35	D	1433	-	57,57,57	1.58	6 (10%)	71,78,78	1.67	15 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C35	B	1433	-	-	12/59/61/61	0/3/3/3
3	C35	D	1433	-	-	10/59/61/61	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1433	C35	N10-N9	-7.14	1.23	1.39
3	D	1433	C35	N10-N9	-7.01	1.24	1.39
3	B	1433	C35	C32-N10	-5.86	1.32	1.43
3	D	1433	C35	C32-N10	-5.18	1.33	1.43
3	B	1433	C35	C28-C29	5.17	1.53	1.49
3	D	1433	C35	C28-C29	4.88	1.53	1.49
3	D	1433	C35	C31-C30	3.69	1.55	1.49
3	B	1433	C35	C31-C30	3.10	1.54	1.49
3	B	1433	C35	C30-N10	-2.97	1.33	1.37
3	D	1433	C35	C30-N10	-2.36	1.34	1.37
3	B	1433	C35	C27-N5	2.23	1.34	1.28
3	D	1433	C35	C27-N5	2.02	1.33	1.28

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1433	C35	N9-C29-N11	-5.02	109.71	115.38
3	D	1433	C35	C25-C26-N5	-4.85	102.09	110.67
3	D	1433	C35	N9-C29-N11	-4.78	109.97	115.38
3	B	1433	C35	C28-C29-N11	3.94	128.57	123.32
3	D	1433	C35	C5-C4-C1	3.59	122.06	118.38
3	D	1433	C35	C28-C29-N11	3.47	127.94	123.32
3	D	1433	C35	C31-C30-N10	3.47	128.22	123.92
3	D	1433	C35	O5-C28-C29	-3.39	116.95	121.40
3	D	1433	C35	C23-N8-C28	-3.04	116.88	122.00
3	B	1433	C35	C32-N10-N9	3.03	123.07	118.67
3	B	1433	C35	C5-C4-C1	3.00	121.46	118.38
3	D	1433	C35	C12-C11-C10	2.93	117.19	111.64
3	B	1433	C35	C31-C30-N11	2.93	127.95	124.96
3	D	1433	C35	C2-C1-C4	-2.87	119.03	122.80
3	D	1433	C35	C32-N10-N9	2.85	122.80	118.67
3	B	1433	C35	C12-C11-N3	2.75	117.01	111.35
3	B	1433	C35	F1-C1-C4	2.71	122.89	118.55
3	D	1433	C35	C33-C32-N10	-2.51	115.95	119.72
3	D	1433	C35	C37-C32-N10	2.45	123.42	119.72
3	D	1433	C35	N7-C27-N6	2.36	121.39	118.21
3	B	1433	C35	C10-C11-N3	-2.35	103.94	110.32
3	B	1433	C35	C4-C5-C6	-2.31	117.96	121.00
3	B	1433	C35	C2-C1-C4	-2.22	119.89	122.80
3	D	1433	C35	C36-C35-CL	2.21	122.62	119.36
3	B	1433	C35	C7-C6-C3	-2.18	116.85	120.90
3	D	1433	C35	C34-C35-CL	-2.12	116.23	119.36
3	B	1433	C35	O2-C10-N2	2.02	126.57	122.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1433	C35	N8-C23-C24-C25
3	B	1433	C35	C22-C23-C24-C25
3	D	1433	C35	N3-C11-C12-C15
3	D	1433	C35	N3-C11-C12-C13
3	D	1433	C35	C10-C11-C12-C15
3	D	1433	C35	C10-C11-C12-C13
3	D	1433	C35	C24-C25-C26-N5
3	B	1433	C35	C10-C11-C12-C13
3	B	1433	C35	C15-C12-C13-C14
3	B	1433	C35	N3-C11-C12-C15
3	B	1433	C35	N3-C11-C12-C13

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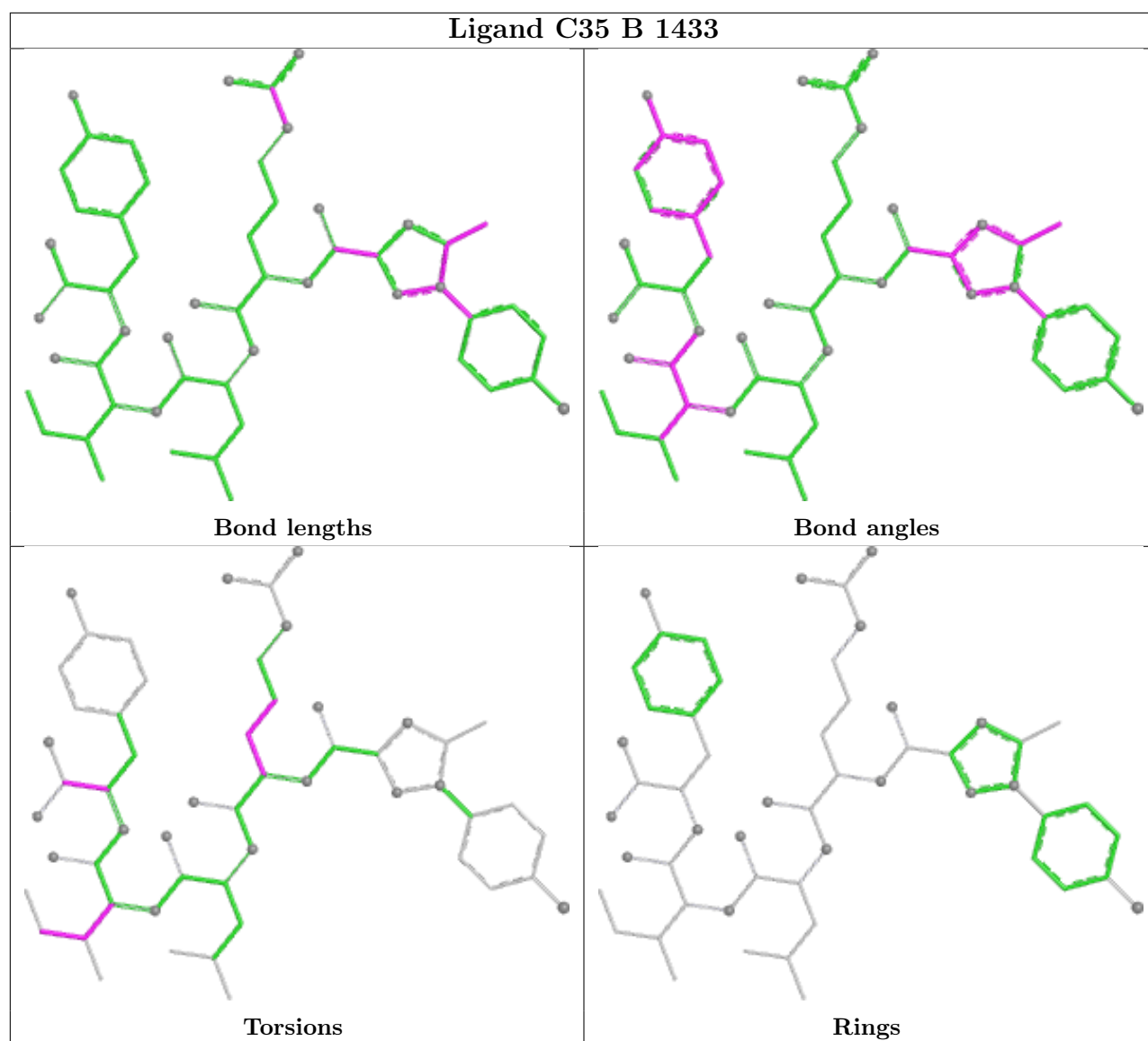
Mol	Chain	Res	Type	Atoms
3	B	1433	C35	N2-C8-C9-O1
3	B	1433	C35	C11-C12-C13-C14
3	B	1433	C35	C23-C24-C25-C26
3	B	1433	C35	C10-C11-C12-C15
3	B	1433	C35	N2-C8-C9-N1
3	D	1433	C35	N8-C28-C29-N9
3	D	1433	C35	O5-C28-C29-N11
3	D	1433	C35	O5-C28-C29-N9
3	D	1433	C35	C22-C23-C24-C25
3	B	1433	C35	C7-C8-C9-O1
3	D	1433	C35	N8-C23-C24-C25

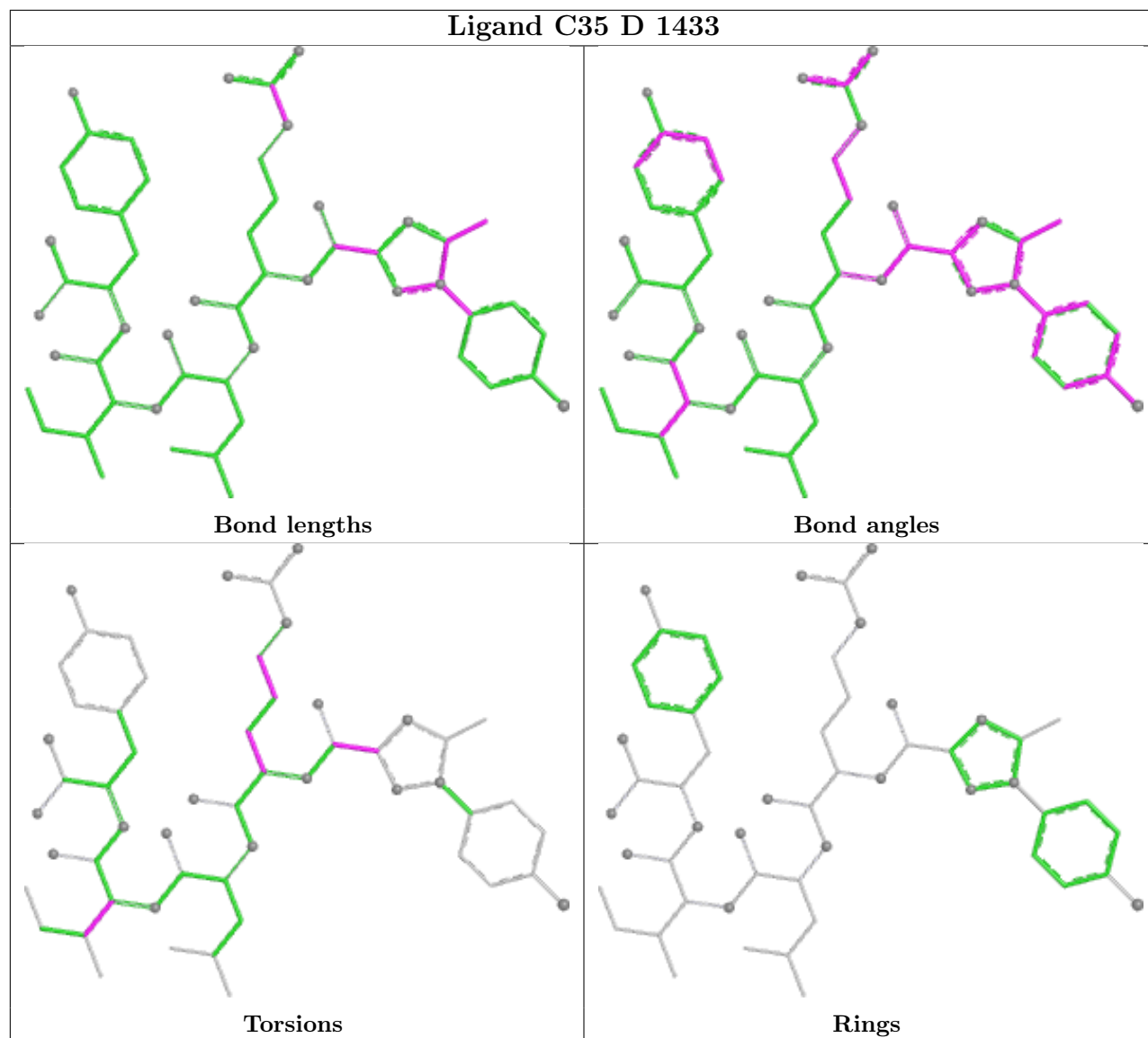
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1433	C35	4	1
3	D	1433	C35	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 [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, 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	296/298 (99%)	-0.62	3 (1%) 79 76	31, 50, 89, 126	0
1	C	297/298 (99%)	-0.68	5 (1%) 69 64	31, 47, 92, 126	0
2	B	258/259 (99%)	-0.73	2 (0%) 82 80	31, 48, 74, 122	0
2	D	258/259 (99%)	-0.74	0 100 100	30, 49, 79, 117	0
All	All	1109/1114 (99%)	-0.69	10 (0%) 81 78	30, 49, 87, 126	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	3.2
1	C	39	THR	3.0
2	B	175	VAL	2.6
1	A	159	TYR	2.4
1	C	159	TYR	2.4
1	A	14	THR	2.4
1	C	15	TYR	2.3
1	C	38	ASP	2.3
1	C	13	GLY	2.2
2	B	178	TYR	2.1

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](#)

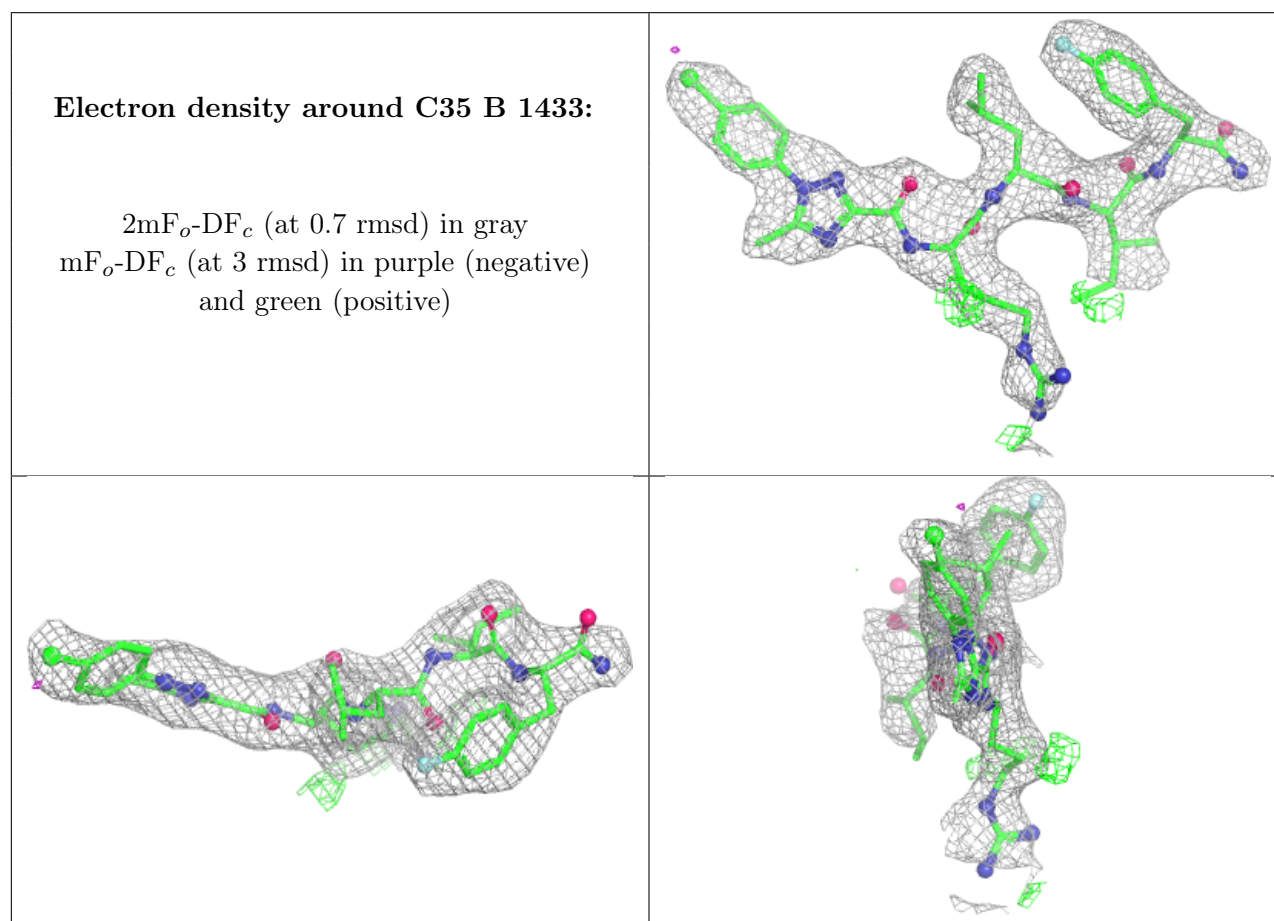
There are no oligosaccharides in this entry.

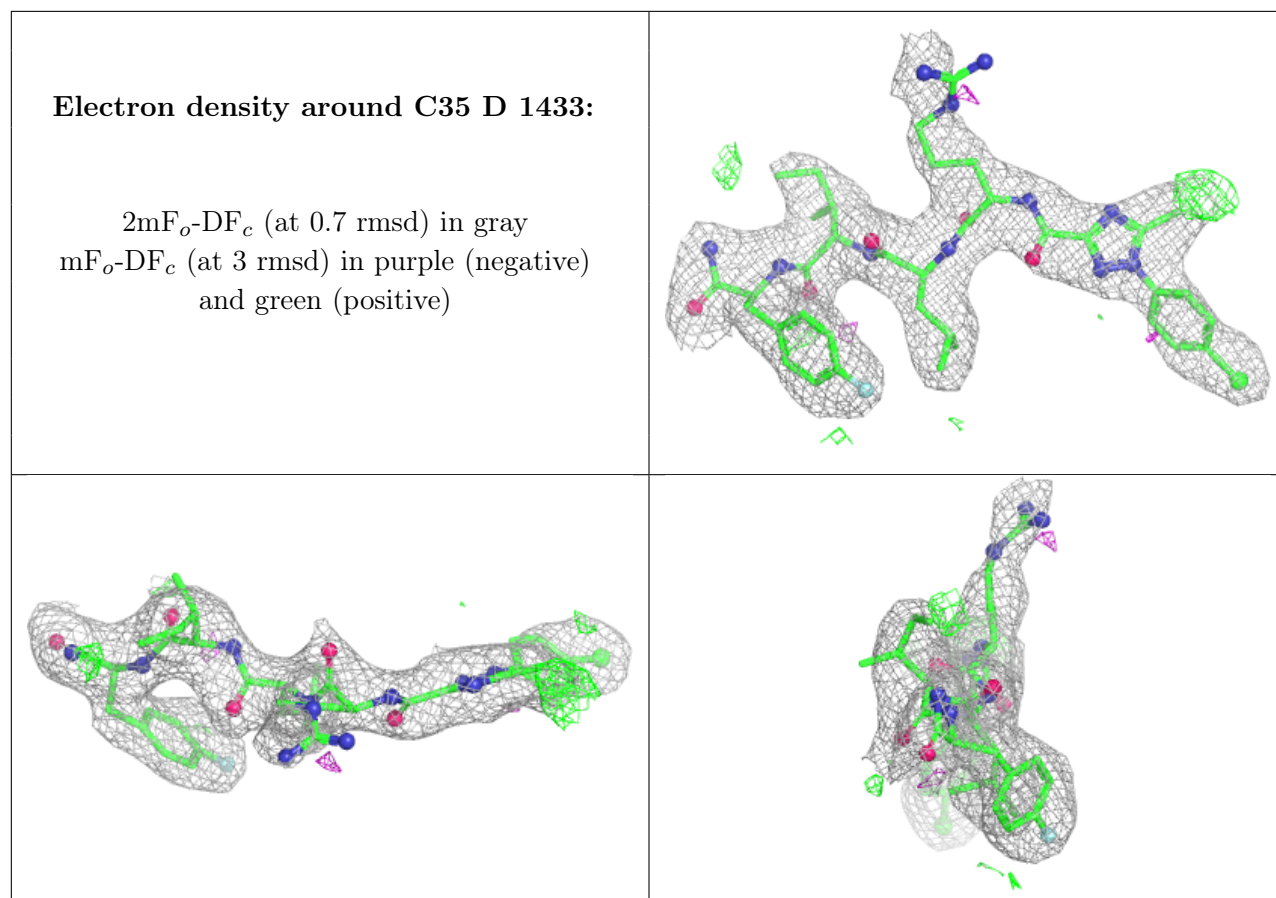
6.4 Ligands ⓘ

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
3	C35	B	1433	55/55	0.92	0.09	27,50,86,93	55
3	C35	D	1433	55/55	0.92	0.09	38,62,96,100	0

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





6.5 Other polymers ⓘ

There are no such residues in this entry.