Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 11:18 am GMT

PDB ID	:	1E3K
Title	:	Human Progesteron Receptor Ligand Binding Domain in complex with the ligand metribolone (R1881)
Authors	:	Matias, P.M.; Donner, P.; Coelho, R.; Thomaz, M.; Peixoto, C.; Macedo, S.; Otto, N.; Joschko, S.; Scholz, P.; Wegg, A.; Basler, S.; Schafer, M.; Egner, U.; Carrondo, M.A.
Deposited on	:	2000-06-19
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

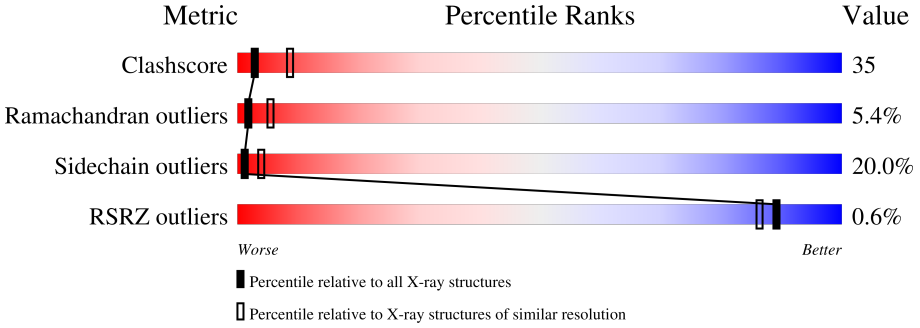
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	21% 40% 28% 9% •
1	B	258	% 18% 41% 30% 7% •

2 Entry composition (i)

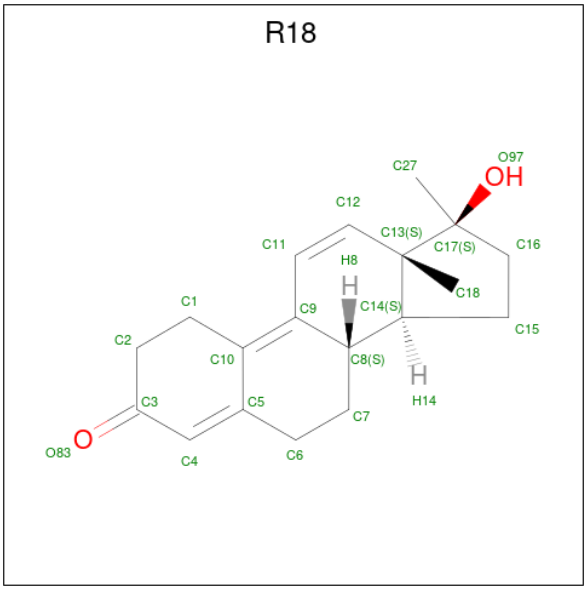
There are 3 unique types of molecules in this entry. The entry contains 4070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROGESTERONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	2010	1305	334	357	14	0	0	0
1	B	249	2017	1308	334	361	14	0	0	0

- Molecule 2 is (17BETA)-17-HYDROXY-17-METHYLESTRA-4,9,11-TRIEN-3-ONE (three-letter code: R18) (formula: $C_{19}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	21	19	2	0	0
2	B	1	21	19	2	0	0

- Molecule 3 is water.

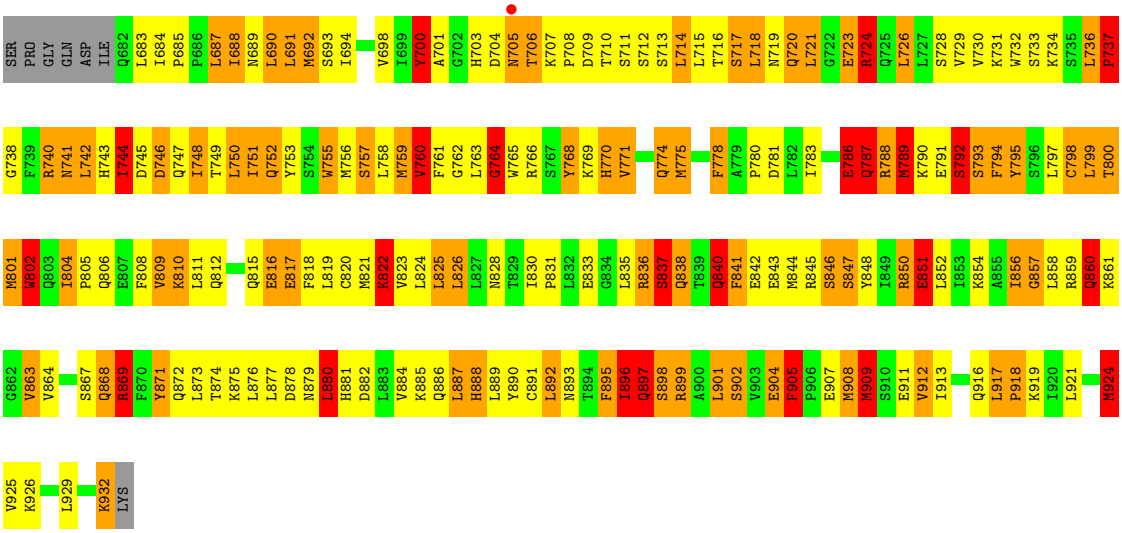
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

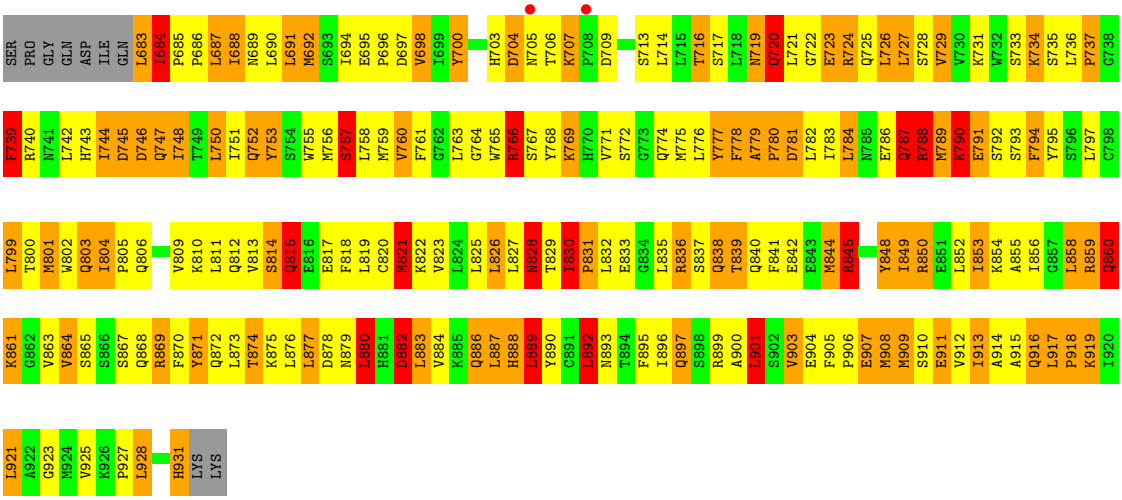
• Molecule 1: PROGESTERONE RECEPTOR

Chain A: 21% 40% 28% 9%



• Molecule 1: PROGESTERONE RECEPTOR

Chain B: % 18% 41% 30% 7%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.40Å 65.01Å 71.18Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	12.50 – 2.80 12.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	67.0 (12.50-2.80) 67.2 (12.45-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.37 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.343 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4070	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: R18

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	1.14	2/2053 (0.1%)	3.14	231/2778 (8.3%)
1	B	1.09	5/2060 (0.2%)	3.06	202/2786 (7.3%)
All	All	1.12	7/4113 (0.2%)	3.10	433/5564 (7.8%)

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	4
1	B	0	3
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	735	SER	CB-OG	-7.38	1.32	1.42
1	B	907	GLU	CD-OE2	6.29	1.32	1.25
1	A	907	GLU	CD-OE2	-6.06	1.19	1.25
1	B	904	GLU	CD-OE2	6.03	1.32	1.25
1	A	837	SER	CB-OG	-5.85	1.34	1.42
1	B	757	SER	CB-OG	5.84	1.49	1.42
1	B	850	ARG	CZ-NH2	5.09	1.39	1.33

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	869	ARG	CD-NE-CZ	37.35	175.90	123.60
1	A	899	ARG	NE-CZ-NH2	-36.63	101.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	869	ARG	NE-CZ-NH2	27.84	134.22	120.30
1	A	778	PHE	CB-CG-CD1	24.35	137.84	120.80
1	B	850	ARG	NE-CZ-NH2	-22.91	108.85	120.30
1	A	842	GLU	CA-CB-CG	21.24	160.13	113.40
1	B	850	ARG	NE-CZ-NH1	20.12	130.36	120.30
1	A	869	ARG	NE-CZ-NH1	19.88	130.24	120.30
1	B	845	ARG	CG-CD-NE	19.71	153.20	111.80
1	A	788	ARG	NE-CZ-NH2	-18.89	110.85	120.30
1	B	766	ARG	NE-CZ-NH2	18.56	129.58	120.30
1	A	753	TYR	CB-CG-CD2	-17.71	110.37	121.00
1	B	734	LYS	CB-CG-CD	16.51	154.53	111.60
1	A	845	ARG	CD-NE-CZ	16.38	146.53	123.60
1	A	793	SER	C-N-CA	15.79	161.19	121.70
1	B	850	ARG	CD-NE-CZ	15.78	145.69	123.60
1	A	904	GLU	OE1-CD-OE2	15.55	141.97	123.30
1	B	724	ARG	NE-CZ-NH1	15.53	128.07	120.30
1	B	740	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	A	753	TYR	CG-CD1-CE1	-14.85	109.42	121.30
1	B	911	GLU	OE1-CD-OE2	-14.59	105.80	123.30
1	A	724	ARG	NE-CZ-NH2	14.43	127.52	120.30
1	B	724	ARG	NE-CZ-NH2	-14.19	113.21	120.30
1	A	899	ARG	CD-NE-CZ	13.95	143.13	123.60
1	A	845	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	850	ARG	NE-CZ-NH2	-13.78	113.41	120.30
1	B	845	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	B	766	ARG	NE-CZ-NH1	-13.42	113.59	120.30
1	B	704	ASP	CB-CG-OD1	12.83	129.85	118.30
1	A	878	ASP	CB-CG-OD1	12.82	129.84	118.30
1	B	892	LEU	CA-CB-CG	12.71	144.52	115.30
1	A	778	PHE	CB-CG-CD2	-12.46	112.08	120.80
1	A	899	ARG	NH1-CZ-NH2	12.42	133.06	119.40
1	B	878	ASP	CB-CG-OD1	12.34	129.41	118.30
1	A	907	GLU	OE1-CD-OE2	-11.93	108.98	123.30
1	B	845	ARG	CD-NE-CZ	11.88	140.23	123.60
1	B	859	ARG	CD-NE-CZ	11.85	140.19	123.60
1	A	850	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	878	ASP	CA-CB-CG	11.60	138.92	113.40
1	A	812	GLN	CA-CB-CG	11.25	138.15	113.40
1	A	911	GLU	OE1-CD-OE2	-11.24	109.81	123.30
1	A	869	ARG	NH1-CZ-NH2	-11.13	107.16	119.40
1	B	836	ARG	NE-CZ-NH1	-11.08	114.76	120.30
1	B	724	ARG	CD-NE-CZ	11.07	139.09	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	732	TRP	CD1-NE1-CE2	10.99	118.89	109.00
1	B	899	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	746	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	B	753	TYR	CB-CG-CD1	10.51	127.31	121.00
1	B	709	ASP	CB-CG-OD1	10.46	127.71	118.30
1	B	775	MET	CA-CB-CG	10.41	130.99	113.30
1	A	869	ARG	CD-NE-CZ	10.31	138.04	123.60
1	A	905	PHE	CB-CG-CD1	10.31	128.02	120.80
1	A	724	ARG	NE-CZ-NH1	-10.23	115.18	120.30
1	A	766	ARG	CD-NE-CZ	10.06	137.68	123.60
1	A	836	ARG	CD-NE-CZ	9.94	137.51	123.60
1	B	766	ARG	CD-NE-CZ	9.71	137.20	123.60
1	A	912	VAL	CG1-CB-CG2	-9.68	95.42	110.90
1	B	844	MET	O-C-N	9.51	137.92	122.70
1	B	726	LEU	CA-CB-CG	9.47	137.09	115.30
1	A	787	GLN	CB-CG-CD	9.39	136.01	111.60
1	B	753	TYR	CG-CD2-CE2	9.36	128.79	121.30
1	A	841	PHE	CD1-CE1-CZ	-9.30	108.94	120.10
1	A	899	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	877	LEU	CB-CG-CD1	-9.27	95.24	111.00
1	A	887	LEU	CB-CG-CD1	9.26	126.74	111.00
1	A	753	TYR	CD1-CE1-CZ	9.21	128.09	119.80
1	A	904	GLU	N-CA-CB	-9.20	94.03	110.60
1	A	890	TYR	CB-CG-CD1	9.20	126.52	121.00
1	B	687	LEU	CA-CB-CG	9.18	136.41	115.30
1	A	816	GLU	OE1-CD-OE2	-9.15	112.32	123.30
1	A	732	TRP	N-CA-CB	9.14	127.06	110.60
1	B	869	ARG	NH1-CZ-NH2	-9.14	109.35	119.40
1	A	794	PHE	N-CA-CB	-9.10	94.21	110.60
1	A	758	LEU	C-N-CA	9.07	144.37	121.70
1	A	851	GLU	OE1-CD-OE2	-9.03	112.47	123.30
1	A	850	ARG	CD-NE-CZ	9.01	136.21	123.60
1	B	899	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	B	845	ARG	CA-CB-CG	8.82	132.81	113.40
1	B	845	ARG	NH1-CZ-NH2	-8.81	109.71	119.40
1	B	735	SER	CB-CA-C	-8.80	93.37	110.10
1	B	878	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	890	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	B	819	LEU	CB-CG-CD2	8.79	125.95	111.00
1	B	778	PHE	CB-CG-CD2	-8.73	114.69	120.80
1	A	789	MET	CA-CB-CG	8.63	127.97	113.30
1	B	700	TYR	CB-CG-CD1	-8.62	115.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	788	ARG	N-CA-CB	-8.62	95.09	110.60
1	A	751	ILE	O-C-N	-8.60	108.95	122.70
1	A	926	LYS	CD-CE-NZ	8.55	131.37	111.70
1	B	879	ASN	CB-CG-OD1	-8.53	104.55	121.60
1	A	787	GLN	CA-CB-CG	8.52	132.13	113.40
1	B	683	LEU	CA-C-O	8.52	137.98	120.10
1	A	912	VAL	CA-CB-CG2	8.50	123.65	110.90
1	B	786	GLU	OE1-CD-OE2	8.49	133.49	123.30
1	A	749	THR	OG1-CB-CG2	8.40	129.31	110.00
1	A	752	GLN	CG-CD-OE1	8.36	138.33	121.60
1	A	819	LEU	O-C-N	-8.32	109.38	122.70
1	A	840	GLN	CB-CG-CD	8.32	133.23	111.60
1	A	732	TRP	CA-CB-CG	8.29	129.46	113.70
1	B	745	ASP	N-CA-CB	-8.26	95.73	110.60
1	A	905	PHE	CB-CG-CD2	-8.24	115.03	120.80
1	A	871	TYR	CB-CG-CD1	-8.24	116.06	121.00
1	A	734	LYS	O-C-N	-8.23	109.53	122.70
1	B	747	GLN	CA-CB-CG	8.19	131.41	113.40
1	A	723	GLU	OE1-CD-OE2	8.15	133.08	123.30
1	A	842	GLU	CB-CA-C	8.14	126.68	110.40
1	B	911	GLU	CA-CB-CG	8.12	131.27	113.40
1	B	753	TYR	CA-C-N	8.10	135.02	117.20
1	B	899	ARG	CD-NE-CZ	8.08	134.91	123.60
1	A	882	ASP	CB-CG-OD1	-8.02	111.08	118.30
1	A	826	LEU	CB-CG-CD2	8.00	124.61	111.00
1	A	770	HIS	CA-CB-CG	7.95	127.11	113.60
1	A	752	GLN	CG-CD-NE2	-7.95	97.63	116.70
1	B	709	ASP	CA-CB-CG	7.93	130.85	113.40
1	A	816	GLU	CG-CD-OE1	7.93	134.16	118.30
1	A	850	ARG	CA-CB-CG	7.91	130.81	113.40
1	A	759	MET	CA-CB-CG	7.89	126.71	113.30
1	B	869	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	760	VAL	O-C-N	-7.84	110.15	122.70
1	A	724	ARG	CG-CD-NE	7.82	128.21	111.80
1	B	729	VAL	CA-CB-CG2	-7.80	99.20	110.90
1	A	878	ASP	OD1-CG-OD2	-7.79	108.49	123.30
1	A	924	MET	C-N-CA	7.78	141.15	121.70
1	A	792	SER	CA-C-O	7.73	136.34	120.10
1	B	809	VAL	CA-CB-CG2	7.69	122.43	110.90
1	B	684	ILE	N-CA-CB	7.65	128.39	110.80
1	B	780	PRO	CA-N-CD	-7.61	100.84	111.50
1	A	732	TRP	NE1-CE2-CD2	-7.58	99.72	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	753	TYR	CD1-CG-CD2	7.52	126.18	117.90
1	B	745	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	897	GLN	CB-CG-CD	7.49	131.08	111.60
1	B	889	LEU	CB-CG-CD2	-7.46	98.32	111.00
1	A	798	CYS	CA-CB-SG	7.36	127.25	114.00
1	A	721	LEU	C-N-CA	7.36	137.75	122.30
1	B	814	SER	N-CA-CB	-7.36	99.47	110.50
1	A	768	TYR	CB-CG-CD1	7.35	125.41	121.00
1	B	897	GLN	OE1-CD-NE2	7.35	138.80	121.90
1	B	775	MET	CA-C-N	7.28	133.21	117.20
1	B	880	LEU	N-CA-CB	-7.26	95.88	110.40
1	B	813	VAL	CA-C-N	-7.25	101.24	117.20
1	A	716	THR	CA-CB-CG2	7.24	122.54	112.40
1	B	888	HIS	CA-C-O	7.20	135.21	120.10
1	A	774	GLN	C-N-CA	7.16	139.60	121.70
1	B	871	TYR	CB-CG-CD2	7.15	125.29	121.00
1	B	766	ARG	CG-CD-NE	7.13	126.78	111.80
1	B	858	LEU	N-CA-CB	-7.12	96.15	110.40
1	A	766	ARG	CA-CB-CG	7.11	129.04	113.40
1	A	721	LEU	CA-CB-CG	-7.10	98.96	115.30
1	B	829	THR	CA-C-N	7.10	132.81	117.20
1	B	683	LEU	O-C-N	-7.08	111.38	122.70
1	B	911	GLU	CG-CD-OE2	7.08	132.45	118.30
1	B	812	GLN	C-N-CA	7.07	139.38	121.70
1	A	932	LYS	CA-CB-CG	7.07	128.96	113.40
1	A	766	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	758	LEU	O-C-N	-6.99	111.52	122.70
1	A	700	TYR	CB-CG-CD2	6.98	125.19	121.00
1	B	899	ARG	CA-CB-CG	6.93	128.65	113.40
1	A	822	LYS	CB-CA-C	6.91	124.22	110.40
1	A	792	SER	O-C-N	-6.90	111.66	122.70
1	B	813	VAL	CA-C-O	6.90	134.58	120.10
1	B	871	TYR	CB-CG-CD1	-6.89	116.86	121.00
1	A	726	LEU	N-CA-CB	-6.87	96.66	110.40
1	A	737	PRO	O-C-N	-6.86	111.54	123.20
1	A	746	ASP	N-CA-CB	-6.84	98.29	110.60
1	A	750	LEU	CB-CG-CD1	6.79	122.55	111.00
1	A	908	MET	C-N-CA	6.78	138.64	121.70
1	B	790	LYS	CD-CE-NZ	6.76	127.25	111.70
1	A	874	THR	CA-C-N	6.75	132.05	117.20
1	A	901	LEU	CB-CG-CD1	6.75	122.47	111.00
1	A	732	TRP	NE1-CE2-CZ2	6.74	137.81	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	821	MET	CA-CB-CG	6.74	124.76	113.30
1	B	761	PHE	CG-CD1-CE1	-6.74	113.39	120.80
1	A	752	GLN	N-CA-CB	6.73	122.71	110.60
1	B	826	LEU	CA-C-O	-6.72	106.00	120.10
1	A	692	MET	N-CA-CB	6.68	122.63	110.60
1	A	747	GLN	OE1-CD-NE2	-6.68	106.55	121.90
1	B	799	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	841	PHE	CZ-CE2-CD2	-6.64	112.13	120.10
1	A	723	GLU	O-C-N	-6.62	112.11	122.70
1	B	698	VAL	CB-CA-C	6.61	123.95	111.40
1	A	817	GLU	CA-CB-CG	6.61	127.93	113.40
1	B	810	LYS	CB-CA-C	6.60	123.59	110.40
1	B	791	GLU	CB-CG-CD	6.59	132.00	114.20
1	B	882	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	778	PHE	CD1-CG-CD2	-6.59	109.74	118.30
1	A	846	SER	CA-CB-OG	-6.59	93.41	111.20
1	A	851	GLU	CG-CD-OE2	6.58	131.47	118.30
1	B	774	GLN	OE1-CD-NE2	6.57	137.00	121.90
1	B	819	LEU	CA-C-N	6.56	131.64	117.20
1	B	790	LYS	CB-CG-CD	6.55	128.64	111.60
1	B	704	ASP	N-CA-CB	6.55	122.39	110.60
1	B	723	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	723	GLU	CG-CD-OE2	6.52	131.35	118.30
1	B	842	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	A	848	TYR	CA-C-N	6.51	131.53	117.20
1	A	736	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	A	760	VAL	CA-CB-CG2	-6.50	101.16	110.90
1	B	842	GLU	CA-CB-CG	6.49	127.68	113.40
1	A	802	TRP	CA-CB-CG	-6.47	101.40	113.70
1	A	911	GLU	CA-CB-CG	6.47	127.64	113.40
1	A	833	GLU	CA-CB-CG	6.47	127.64	113.40
1	A	836	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	A	716	THR	CA-CB-OG1	-6.44	95.47	109.00
1	B	859	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	804	ILE	CA-CB-CG1	6.42	123.20	111.00
1	A	778	PHE	C-N-CA	6.42	137.75	121.70
1	A	758	LEU	CA-C-N	6.38	131.24	117.20
1	A	810	LYS	CA-CB-CG	6.36	127.39	113.40
1	A	788	ARG	NH1-CZ-NH2	6.35	126.39	119.40
1	B	853	ILE	CB-CG1-CD1	-6.35	96.12	113.90
1	A	764	GLY	O-C-N	-6.34	112.56	122.70
1	A	879	ASN	OD1-CG-ND2	6.32	136.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	748	ILE	CB-CG1-CD1	6.29	131.51	113.90
1	A	860	GLN	N-CA-CB	6.29	121.92	110.60
1	B	886	GLN	OE1-CD-NE2	6.28	136.34	121.90
1	A	783	ILE	CA-C-N	6.28	131.01	117.20
1	B	828	ASN	CA-C-O	-6.27	106.92	120.10
1	B	923	GLY	O-C-N	-6.27	112.66	122.70
1	B	779	ALA	CB-CA-C	6.23	119.44	110.10
1	B	753	TYR	O-C-N	-6.22	112.75	122.70
1	A	859	ARG	CD-NE-CZ	-6.17	114.95	123.60
1	A	840	GLN	O-C-N	-6.17	112.83	122.70
1	A	905	PHE	O-C-N	-6.17	109.38	121.10
1	B	838	GLN	CB-CA-C	6.16	122.72	110.40
1	B	917	LEU	CB-CA-C	6.15	121.89	110.20
1	B	830	ILE	CA-CB-CG2	-6.15	98.60	110.90
1	A	775	MET	CA-C-O	-6.14	107.20	120.10
1	A	721	LEU	CB-CG-CD2	6.14	121.44	111.00
1	B	752	GLN	C-N-CA	6.14	137.04	121.70
1	A	841	PHE	CE1-CZ-CE2	6.13	131.04	120.00
1	B	801	MET	CA-CB-CG	-6.13	102.88	113.30
1	B	815	GLN	CG-CD-OE1	6.12	133.85	121.60
1	A	718	LEU	CB-CA-C	6.12	121.83	110.20
1	A	757	SER	O-C-N	-6.11	112.92	122.70
1	A	789	MET	N-CA-CB	6.11	121.59	110.60
1	B	914	ALA	N-CA-CB	6.11	118.65	110.10
1	B	849	ILE	C-N-CA	6.09	136.93	121.70
1	B	879	ASN	OD1-CG-ND2	6.08	135.89	121.90
1	A	909	MET	N-CA-CB	-6.08	99.66	110.60
1	A	845	ARG	NH1-CZ-NH2	-6.07	112.73	119.40
1	B	892	LEU	CB-CG-CD1	6.05	121.29	111.00
1	A	742	LEU	O-C-N	-6.05	113.02	122.70
1	A	690	LEU	CB-CA-C	6.04	121.68	110.20
1	A	721	LEU	CB-CA-C	6.04	121.68	110.20
1	B	887	LEU	CB-CG-CD2	6.03	121.25	111.00
1	B	848	TYR	O-C-N	-6.02	113.06	122.70
1	A	809	VAL	CA-CB-CG1	6.02	119.93	110.90
1	B	689	ASN	CB-CG-ND2	-6.01	102.28	116.70
1	B	822	LYS	CB-CA-C	6.01	122.42	110.40
1	B	719	ASN	CB-CG-ND2	-6.01	102.28	116.70
1	A	788	ARG	CA-C-N	5.99	130.38	117.20
1	B	775	MET	CA-C-O	-5.98	107.55	120.10
1	B	812	GLN	O-C-N	-5.97	113.14	122.70
1	B	914	ALA	O-C-N	5.97	132.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	779	ALA	N-CA-CB	-5.96	101.76	110.10
1	A	916	GLN	CB-CA-C	5.95	122.29	110.40
1	A	904	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	B	836	ARG	CA-C-N	5.93	130.24	117.20
1	A	745	ASP	CA-C-O	5.92	132.53	120.10
1	A	774	GLN	O-C-N	-5.92	113.23	122.70
1	B	895	PHE	O-C-N	-5.91	113.25	122.70
1	A	857	GLY	N-CA-C	5.91	127.86	113.10
1	A	691	LEU	O-C-N	-5.90	113.26	122.70
1	A	858	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	882	ASP	OD1-CG-OD2	5.88	134.48	123.30
1	A	778	PHE	CG-CD2-CE2	5.87	127.26	120.80
1	B	901	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	A	756	MET	CA-CB-CG	-5.86	103.33	113.30
1	A	857	GLY	O-C-N	-5.86	113.32	122.70
1	A	745	ASP	O-C-N	-5.85	113.34	122.70
1	A	880	LEU	N-CA-CB	5.85	122.11	110.40
1	B	791	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	A	885	LYS	CD-CE-NZ	-5.85	98.25	111.70
1	B	919	LYS	CA-CB-CG	5.85	126.27	113.40
1	B	848	TYR	CG-CD2-CE2	-5.85	116.62	121.30
1	B	746	ASP	O-C-N	-5.84	113.35	122.70
1	A	740	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	755	TRP	CA-CB-CG	-5.84	102.60	113.70
1	B	912	VAL	O-C-N	-5.84	113.35	122.70
1	A	924	MET	O-C-N	-5.82	113.39	122.70
1	B	820	CYS	N-CA-CB	-5.82	100.13	110.60
1	A	856	ILE	CB-CG1-CD1	5.81	130.17	113.90
1	B	740	ARG	NH1-CZ-NH2	5.81	125.79	119.40
1	B	917	LEU	N-CA-CB	-5.81	98.78	110.40
1	A	825	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	719	ASN	N-CA-CB	-5.80	100.16	110.60
1	A	795	TYR	N-CA-C	-5.79	95.36	111.00
1	B	826	LEU	O-C-N	5.78	131.95	122.70
1	A	815	GLN	CB-CG-CD	-5.78	96.57	111.60
1	B	691	LEU	CB-CA-C	5.78	121.17	110.20
1	B	724	ARG	CG-CD-NE	5.78	123.93	111.80
1	A	757	SER	CB-CA-C	5.76	121.04	110.10
1	A	760	VAL	CA-CB-CG1	5.75	119.52	110.90
1	A	753	TYR	CA-C-N	5.74	129.83	117.20
1	B	753	TYR	CZ-CE2-CD2	-5.74	114.64	119.80
1	B	776	LEU	CA-CB-CG	-5.74	102.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	890	TYR	CB-CG-CD2	5.74	124.44	121.00
1	B	845	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	831	PRO	CA-N-CD	-5.73	103.47	111.50
1	B	919	LYS	CB-CG-CD	5.73	126.50	111.60
1	B	907	GLU	CG-CD-OE2	-5.73	106.84	118.30
1	B	931	HIS	CA-C-O	5.72	132.12	120.10
1	B	806	GLN	CB-CA-C	5.72	121.84	110.40
1	A	729	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	B	836	ARG	O-C-N	-5.71	113.57	122.70
1	A	817	GLU	N-CA-CB	5.69	120.85	110.60
1	B	812	GLN	CA-CB-CG	5.66	125.85	113.40
1	A	801	MET	O-C-N	-5.66	113.65	122.70
1	A	860	GLN	CA-CB-CG	5.66	125.84	113.40
1	A	859	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	774	GLN	CB-CA-C	5.65	121.69	110.40
1	A	742	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	726	LEU	CB-CA-C	-5.62	99.52	110.20
1	A	758	LEU	O-C-N	-5.62	113.71	122.70
1	A	774	GLN	N-CA-CB	-5.60	100.52	110.60
1	B	849	ILE	O-C-N	-5.59	113.75	122.70
1	A	721	LEU	O-C-N	-5.59	113.70	123.20
1	B	790	LYS	CA-CB-CG	5.59	125.70	113.40
1	A	888	HIS	CA-C-O	5.59	131.84	120.10
1	B	777	TYR	CB-CG-CD2	5.58	124.35	121.00
1	A	738	GLY	CA-C-O	-5.58	110.55	120.60
1	B	769	LYS	CB-CA-C	-5.57	99.25	110.40
1	B	771	VAL	CA-CB-CG2	5.56	119.24	110.90
1	B	787	GLN	N-CA-CB	-5.55	100.62	110.60
1	A	905	PHE	CD1-CE1-CZ	5.54	126.75	120.10
1	A	924	MET	CB-CA-C	5.52	121.44	110.40
1	A	751	ILE	CG1-CB-CG2	5.52	123.54	111.40
1	A	875	LYS	CA-CB-CG	5.52	125.54	113.40
1	A	797	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	839	THR	CA-CB-CG2	5.51	120.12	112.40
1	A	742	LEU	CA-C-O	5.51	131.68	120.10
1	A	838	GLN	O-C-N	-5.51	113.88	122.70
1	A	842	GLU	N-CA-CB	-5.49	100.71	110.60
1	B	903	VAL	CA-CB-CG2	5.48	119.12	110.90
1	B	844	MET	CA-C-O	-5.48	108.59	120.10
1	A	800	THR	CA-CB-OG1	-5.48	97.50	109.00
1	B	788	ARG	CA-CB-CG	-5.48	101.35	113.40
1	B	794	PHE	CB-CA-C	5.47	121.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	683	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	760	VAL	C-N-CA	5.46	135.34	121.70
1	A	793	SER	O-C-N	-5.45	113.98	122.70
1	B	803	GLN	N-CA-CB	-5.45	100.80	110.60
1	B	750	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	845	ARG	N-CA-CB	5.43	120.37	110.60
1	B	907	GLU	N-CA-C	5.43	125.65	111.00
1	B	913	ILE	CA-CB-CG1	-5.43	100.69	111.00
1	B	753	TYR	N-CA-CB	5.41	120.33	110.60
1	B	782	LEU	N-CA-CB	5.40	121.19	110.40
1	B	873	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	889	LEU	O-C-N	-5.38	114.09	122.70
1	A	892	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	821	MET	N-CA-CB	5.37	120.27	110.60
1	A	786	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	A	833	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	B	900	ALA	CB-CA-C	5.35	118.13	110.10
1	A	904	GLU	CB-CA-C	5.34	121.09	110.40
1	B	897	GLN	CG-CD-OE1	-5.34	110.91	121.60
1	A	745	ASP	C-N-CA	5.34	135.06	121.70
1	A	769	LYS	CD-CE-NZ	5.34	123.99	111.70
1	B	819	LEU	O-C-N	-5.34	114.16	122.70
1	B	739	PHE	O-C-N	-5.33	114.17	122.70
1	A	896	ILE	CA-C-N	5.31	128.88	117.20
1	B	778	PHE	CD1-CG-CD2	5.31	125.20	118.30
1	A	925	VAL	CB-CA-C	-5.30	101.32	111.40
1	A	868	GLN	CB-CG-CD	5.30	125.38	111.60
1	A	833	GLU	CG-CD-OE2	5.27	128.84	118.30
1	B	692	MET	N-CA-CB	5.27	120.09	110.60
1	A	720	GLN	CA-CB-CG	5.27	124.99	113.40
1	B	727	LEU	N-CA-CB	-5.27	99.87	110.40
1	B	823	VAL	O-C-N	5.26	131.12	122.70
1	A	740	ARG	CB-CA-C	-5.25	99.90	110.40
1	A	688	ILE	CA-C-N	5.25	128.74	117.20
1	A	877	LEU	CB-CG-CD2	5.24	119.91	111.00
1	B	781	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	786	GLU	CB-CA-C	-5.24	99.93	110.40
1	A	887	LEU	O-C-N	-5.23	114.33	122.70
1	A	700	TYR	CG-CD1-CE1	5.23	125.48	121.30
1	B	775	MET	CG-SD-CE	-5.23	91.84	100.20
1	A	804	ILE	N-CA-CB	5.22	122.80	110.80
1	B	782	LEU	CA-C-O	-5.21	109.16	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	688	ILE	CG1-CB-CG2	-5.20	99.95	111.40
1	A	823	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	745	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	907	GLU	CG-CD-OE2	5.19	128.68	118.30
1	B	727	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	B	836	ARG	C-N-CA	5.18	134.66	121.70
1	A	751	ILE	C-N-CA	5.18	134.65	121.70
1	B	753	TYR	CD1-CG-CD2	-5.18	112.20	117.90
1	B	768	TYR	CA-C-O	-5.18	109.22	120.10
1	A	732	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	770	HIS	N-CA-CB	5.16	119.89	110.60
1	A	711	SER	CB-CA-C	5.16	119.90	110.10
1	B	700	TYR	CB-CG-CD2	5.16	124.09	121.00
1	A	911	GLU	O-C-N	5.15	130.94	122.70
1	B	921	LEU	N-CA-CB	5.15	120.70	110.40
1	A	775	MET	N-CA-CB	5.14	119.85	110.60
1	A	712	SER	N-CA-CB	-5.13	102.80	110.50
1	B	928	LEU	CB-CA-C	5.12	119.94	110.20
1	B	860	GLN	N-CA-CB	5.12	119.82	110.60
1	A	795	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	824	LEU	CA-C-O	-5.11	109.36	120.10
1	A	876	LEU	CB-CG-CD2	5.11	119.69	111.00
1	B	826	LEU	CB-CG-CD1	5.11	119.69	111.00
1	A	744	ILE	N-CA-CB	5.11	122.55	110.80
1	B	845	ARG	CB-CG-CD	5.10	124.86	111.60
1	B	737	PRO	CB-CA-C	5.10	124.74	112.00
1	B	698	VAL	CA-CB-CG2	5.09	118.54	110.90
1	B	768	TYR	CA-C-N	5.09	128.39	117.20
1	A	805	PRO	N-CA-CB	5.09	109.41	103.30
1	A	700	TYR	O-C-N	-5.08	114.57	122.70
1	B	890	TYR	O-C-N	5.08	130.83	122.70
1	A	911	GLU	CB-CA-C	5.08	120.56	110.40
1	B	704	ASP	OD1-CG-OD2	-5.08	113.65	123.30
1	A	771	VAL	N-CA-CB	5.07	122.66	111.50
1	A	838	GLN	N-CA-CB	5.07	119.72	110.60
1	A	843	GLU	N-CA-CB	5.07	119.72	110.60
1	B	716	THR	CA-C-N	5.07	128.35	117.20
1	A	748	ILE	CB-CG1-CD1	-5.07	99.72	113.90
1	A	820	CYS	CA-C-O	-5.07	109.46	120.10
1	B	716	THR	O-C-N	-5.07	114.59	122.70
1	A	808	PHE	CG-CD2-CE2	5.06	126.37	120.80
1	B	874	THR	CA-C-N	5.06	128.33	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	693	SER	N-CA-CB	5.04	118.07	110.50
1	B	914	ALA	CB-CA-C	-5.04	102.53	110.10
1	A	744	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	A	819	LEU	CB-CA-C	5.03	119.77	110.20
1	B	877	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	B	776	LEU	CB-CG-CD1	5.02	119.54	111.00
1	B	916	GLN	CG-CD-NE2	-5.02	104.65	116.70
1	B	727	LEU	O-C-N	-5.02	114.67	122.70
1	B	783	ILE	O-C-N	-5.01	114.68	122.70
1	A	753	TYR	CG-CD2-CE2	-5.00	117.30	121.30
1	B	683	LEU	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	687	LEU	Mainchain
1	A	792	SER	Peptide
1	A	861	LYS	Peptide
1	A	929	LEU	Peptide
1	B	739	PHE	Mainchain
1	B	861	LYS	Peptide
1	B	915	ALA	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2010	0	2053	125	0
1	B	2017	0	2077	168	0
2	A	21	0	24	5	0
2	B	21	0	24	1	0
3	A	1	0	0	0	0
All	All	4070	0	4178	290	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 35.

All (290) 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:720:GLN:HE21	1:A:724:ARG:NE	1.56	1.03
1:B:784:LEU:HD22	1:B:788:ARG:HD3	1.40	1.01
1:B:721:LEU:HD11	1:B:725:GLN:HE21	1.22	0.98
1:A:825:LEU:HD23	1:A:828:ASN:HD22	1.23	0.98
1:A:720:GLN:HE21	1:A:724:ARG:HE	1.06	0.96
1:B:727:LEU:HG	1:B:908:MET:HE1	1.50	0.91
1:A:752:GLN:HG2	1:A:912:VAL:HG12	1.51	0.90
1:B:800:THR:HA	1:B:803:GLN:NE2	1.93	0.83
1:B:692:MET:SD	1:B:815:GLN:NE2	2.51	0.83
1:B:690:LEU:HD23	1:B:737:PRO:HG3	1.62	0.82
1:A:720:GLN:NE2	1:A:724:ARG:HE	1.79	0.81
1:B:784:LEU:HD22	1:B:788:ARG:CD	2.09	0.81
1:A:726:LEU:O	1:A:730:VAL:HG23	1.81	0.80
1:B:855:ALA:HA	1:B:858:LEU:HD12	1.63	0.78
1:B:830:ILE:HG22	1:B:831:PRO:HD3	1.66	0.77
1:B:753:TYR:HE1	1:B:916:GLN:NE2	1.83	0.77
1:A:868:GLN:O	1:A:872:GLN:HG3	1.86	0.74
1:B:685:PRO:HG2	1:B:688:ILE:HD12	1.67	0.74
1:A:701:ALA:HB2	1:A:721:LEU:HD13	1.68	0.74
1:B:790:LYS:HG3	1:B:791:GLU:HG3	1.69	0.74
1:A:771:VAL:HG21	1:A:775:MET:HB2	1.69	0.74
1:B:721:LEU:HD11	1:B:725:GLN:NE2	2.01	0.73
1:B:814:SER:HB2	1:B:859:ARG:NH1	2.03	0.73
1:A:811:LEU:O	1:A:869:ARG:NH1	2.20	0.73
1:B:690:LEU:CD2	1:B:737:PRO:HG3	2.18	0.73
1:A:825:LEU:HD23	1:A:828:ASN:ND2	2.02	0.73
1:B:917:LEU:N	1:B:918:PRO:HD2	2.04	0.73
1:A:718:LEU:O	2:A:1000:R18:H11	1.88	0.73
1:A:720:GLN:HG3	1:A:724:ARG:HE	1.53	0.73
1:A:892:LEU:HD21	1:B:892:LEU:HD11	1.69	0.72
1:B:744:ILE:O	1:B:748:ILE:HD12	1.90	0.72
1:B:814:SER:HB2	1:B:859:ARG:HH11	1.53	0.72
1:A:792:SER:O	1:A:794:PHE:HB3	1.90	0.72
1:A:685:PRO:HG2	1:A:688:ILE:HD12	1.72	0.71
1:A:752:GLN:CG	1:A:912:VAL:HG12	2.20	0.71
1:B:733:SER:HB2	1:B:739:PHE:CD2	2.25	0.71
1:A:720:GLN:O	1:A:724:ARG:HD2	1.91	0.70
1:B:714:LEU:HD23	1:B:794:PHE:CE2	2.27	0.70
1:A:806:GLN:OE1	1:A:806:GLN:HA	1.91	0.69
1:A:913:ILE:HA	1:A:917:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:ALA:O	1:B:858:LEU:HB2	1.93	0.69
1:B:917:LEU:N	1:B:918:PRO:CD	2.56	0.68
1:B:684:ILE:CG2	1:B:688:ILE:HB	2.22	0.68
1:B:925:VAL:O	1:B:927:PRO:HD3	1.91	0.68
1:A:837:SER:HB3	1:A:840:GLN:OE1	1.93	0.68
1:B:855:ALA:HA	1:B:858:LEU:CD1	2.23	0.68
1:B:757:SER:OG	1:B:825:LEU:HD13	1.93	0.68
1:B:864:VAL:O	1:B:868:GLN:HG3	1.94	0.68
1:A:760:VAL:HG21	1:A:887:LEU:HD11	1.74	0.67
1:A:707:LYS:CB	1:A:708:PRO:HD2	2.24	0.67
1:A:789:MET:HG2	1:A:798:CYS:SG	2.36	0.66
1:A:851:GLU:OE1	1:A:851:GLU:HA	1.94	0.66
1:B:821:MET:HB3	1:B:877:LEU:HD11	1.75	0.66
1:B:876:LEU:O	1:B:876:LEU:HD23	1.95	0.66
1:A:830:ILE:HB	1:A:831:PRO:HD2	1.77	0.66
1:A:893:ASN:OD1	1:B:918:PRO:HG2	1.95	0.66
1:B:685:PRO:HB2	1:B:688:ILE:HG13	1.79	0.65
1:B:883:LEU:O	1:B:886:GLN:HB2	1.97	0.65
1:A:765:TRP:HB2	1:A:818:PHE:CE1	2.32	0.65
1:B:727:LEU:HG	1:B:908:MET:CE	2.26	0.65
1:B:880:LEU:O	1:B:884:VAL:HG23	1.96	0.65
1:B:759:MET:HG2	2:B:1000:R18:H21	1.79	0.63
1:B:889:LEU:H	1:B:921:LEU:HD21	1.63	0.63
1:A:826:LEU:O	1:A:826:LEU:HD12	1.98	0.63
1:A:896:ILE:HD11	1:B:892:LEU:CD1	2.28	0.63
1:A:901:LEU:O	1:A:902:SER:HB2	1.97	0.63
1:B:870:PHE:O	1:B:874:THR:HG23	1.98	0.63
1:A:790:LYS:O	1:A:791:GLU:C	2.37	0.63
1:B:725:GLN:O	1:B:729:VAL:HG23	1.99	0.63
1:B:897:GLN:O	1:B:901:LEU:HG	1.99	0.62
1:B:830:ILE:CG2	1:B:831:PRO:HD3	2.29	0.62
1:B:767:SER:OG	1:B:777:TYR:N	2.29	0.62
1:A:892:LEU:HD23	1:B:918:PRO:HB3	1.81	0.62
1:A:698:VAL:HG21	1:A:780:PRO:HG3	1.82	0.61
1:B:838:GLN:HA	1:B:838:GLN:NE2	2.16	0.61
1:A:860:GLN:HE21	1:A:860:GLN:HA	1.65	0.61
1:A:917:LEU:N	1:A:918:PRO:CD	2.63	0.61
1:B:854:LYS:O	1:B:858:LEU:HG	2.00	0.60
1:A:847:SER:HB2	1:A:850:ARG:NH2	2.16	0.60
1:A:746:ASP:OD2	1:A:835:LEU:HB3	2.02	0.60
1:A:768:TYR:HD1	1:A:809:VAL:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ARG:O	1:B:849:ILE:HG13	2.01	0.60
1:B:837:SER:O	1:B:840:GLN:HB2	2.01	0.60
1:B:797:LEU:HD23	1:B:801:MET:CE	2.31	0.60
1:B:849:ILE:O	1:B:852:LEU:HB3	2.02	0.60
1:B:733:SER:HB2	1:B:739:PHE:HD2	1.67	0.59
1:B:714:LEU:HD23	1:B:794:PHE:CZ	2.37	0.59
1:B:830:ILE:HG21	1:B:835:LEU:CD1	2.33	0.59
1:B:787:GLN:O	1:B:790:LYS:HG2	2.02	0.59
1:A:743:HIS:ND1	1:A:836:ARG:HD3	2.17	0.58
1:B:746:ASP:CB	1:B:835:LEU:HD22	2.33	0.58
1:B:875:LYS:HD3	1:B:931:HIS:HD2	1.67	0.58
1:B:889:LEU:N	1:B:921:LEU:HD21	2.19	0.58
1:A:860:GLN:CG	1:A:869:ARG:HG2	2.34	0.58
1:B:787:GLN:CD	1:B:790:LYS:HE2	2.24	0.58
1:A:852:LEU:O	1:A:856:ILE:HG13	2.04	0.58
1:B:868:GLN:O	1:B:872:GLN:HG3	2.03	0.58
1:B:753:TYR:HE1	1:B:916:GLN:HE21	1.49	0.58
1:B:826:LEU:O	1:B:826:LEU:HG	2.04	0.58
1:A:691:LEU:O	1:A:692:MET:C	2.43	0.57
1:B:765:TRP:HB2	1:B:818:PHE:CE1	2.40	0.57
1:A:684:ILE:HB	1:A:689:ASN:HD21	1.68	0.57
1:B:804:ILE:HB	1:B:805:PRO:HD3	1.87	0.57
1:B:892:LEU:HD12	1:B:896:ILE:HD11	1.86	0.56
1:B:917:LEU:H	1:B:918:PRO:HD2	1.68	0.56
1:B:750:LEU:HD21	1:B:830:ILE:HG23	1.87	0.56
1:B:852:LEU:O	1:B:856:ILE:HG13	2.06	0.56
1:B:684:ILE:HG22	1:B:688:ILE:HB	1.87	0.56
1:B:691:LEU:HD23	1:B:694:ILE:HD11	1.87	0.56
1:B:746:ASP:CG	1:B:835:LEU:HD22	2.26	0.56
1:B:830:ILE:CB	1:B:831:PRO:CD	2.84	0.56
1:A:692:MET:HA	1:A:692:MET:CE	2.35	0.55
1:B:830:ILE:HG21	1:B:835:LEU:HD11	1.87	0.55
1:B:830:ILE:HB	1:B:831:PRO:CD	2.37	0.55
1:B:721:LEU:CD1	1:B:725:GLN:HE21	2.08	0.55
1:B:787:GLN:OE1	1:B:790:LYS:HE2	2.07	0.55
1:A:704:ASP:O	1:A:706:THR:N	2.40	0.55
1:A:860:GLN:HG3	1:A:869:ARG:HG2	1.88	0.55
1:B:763:LEU:O	1:B:764:GLY:C	2.45	0.55
1:B:779:ALA:HB1	1:B:780:PRO:CD	2.37	0.55
1:A:752:GLN:HG2	1:A:912:VAL:CG1	2.32	0.55
1:A:707:LYS:CB	1:A:708:PRO:CD	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:HIS:HD2	1:B:717:SER:OG	1.90	0.54
1:B:767:SER:HG	1:B:777:TYR:N	2.04	0.54
1:B:835:LEU:HB2	1:B:838:GLN:NE2	2.21	0.54
1:A:817:GLU:OE1	1:A:873:LEU:HD11	2.08	0.54
1:B:892:LEU:HD23	1:B:921:LEU:HD12	1.89	0.54
1:B:727:LEU:CG	1:B:908:MET:HE1	2.30	0.54
1:B:841:PHE:CZ	1:B:845:ARG:HG3	2.43	0.54
1:B:830:ILE:HD11	1:B:928:LEU:HD11	1.88	0.54
1:B:700:TYR:CE2	1:B:780:PRO:HG2	2.43	0.54
1:A:755:TRP:CH2	1:A:909:MET:HE2	2.43	0.53
1:B:742:LEU:O	1:B:747:GLN:NE2	2.31	0.53
1:A:869:ARG:O	1:A:872:GLN:HB2	2.08	0.53
1:A:917:LEU:HB2	1:A:918:PRO:HD3	1.89	0.53
1:A:701:ALA:CB	1:A:721:LEU:HD13	2.39	0.52
1:A:897:GLN:HB2	1:A:901:LEU:HD12	1.91	0.52
1:B:837:SER:O	1:B:838:GLN:C	2.47	0.52
1:B:763:LEU:HD22	1:B:778:PHE:CE1	2.45	0.52
1:A:740:ARG:HG3	1:A:741:ASN:ND2	2.25	0.51
1:A:757:SER:HB2	1:A:884:VAL:HG21	1.92	0.51
1:A:690:LEU:HD13	1:A:737:PRO:HG2	1.92	0.51
1:A:800:THR:HG21	1:A:886:GLN:OE1	2.10	0.51
1:B:692:MET:SD	1:B:815:GLN:CD	2.88	0.51
1:B:888:HIS:HB3	1:B:921:LEU:HD21	1.92	0.51
1:A:795:TYR:CZ	1:A:799:LEU:HD21	2.45	0.51
1:B:892:LEU:HD23	1:B:921:LEU:CD1	2.40	0.51
1:B:815:GLN:O	1:B:815:GLN:HG3	2.08	0.51
1:B:837:SER:HB3	1:B:840:GLN:HB2	1.92	0.51
1:A:692:MET:HA	1:A:692:MET:HE3	1.93	0.51
1:A:763:LEU:O	1:A:764:GLY:C	2.48	0.51
1:B:766:ARG:HD2	1:B:777:TYR:CD1	2.46	0.50
1:B:830:ILE:CB	1:B:831:PRO:HD3	2.41	0.50
1:B:736:LEU:HD12	1:B:737:PRO:HD2	1.93	0.50
1:B:892:LEU:CD2	1:B:921:LEU:HD12	2.42	0.50
1:B:742:LEU:HB2	1:B:747:GLN:HG3	1.92	0.50
1:B:814:SER:OG	1:B:817:GLU:HG3	2.11	0.50
1:B:719:ASN:HD22	1:B:905:PHE:HA	1.76	0.50
1:A:838:GLN:O	1:A:841:PHE:HB3	2.12	0.50
1:B:795:TYR:OH	1:B:799:LEU:HD21	2.12	0.50
1:A:740:ARG:HG3	1:A:741:ASN:HD22	1.77	0.50
1:B:766:ARG:HD2	1:B:777:TYR:HD1	1.76	0.49
1:A:917:LEU:N	1:A:918:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASP:OD2	1:A:836:ARG:N	2.45	0.49
1:B:830:ILE:HG21	1:B:835:LEU:HG	1.93	0.49
1:A:720:GLN:HG3	1:A:724:ARG:NE	2.26	0.49
1:B:830:ILE:CD1	1:B:928:LEU:HD11	2.43	0.49
1:B:683:LEU:O	1:B:684:ILE:HG12	2.13	0.49
1:B:719:ASN:O	1:B:722:GLY:N	2.45	0.49
1:A:752:GLN:O	1:A:755:TRP:HD1	1.94	0.49
1:B:830:ILE:HG21	1:B:835:LEU:CG	2.43	0.48
1:A:868:GLN:O	1:A:871:TYR:HB3	2.13	0.48
1:B:685:PRO:HG2	1:B:688:ILE:CD1	2.39	0.48
1:A:804:ILE:HD11	1:A:880:LEU:HD22	1.96	0.48
1:A:723:GLU:CD	1:A:908:MET:HB2	2.34	0.48
1:B:797:LEU:HD23	1:B:801:MET:HE2	1.95	0.48
1:A:895:PHE:O	1:A:898:SER:HB3	2.14	0.47
1:B:716:THR:OG1	1:B:903:VAL:HG13	2.14	0.47
1:B:790:LYS:CG	1:B:791:GLU:N	2.77	0.47
1:A:721:LEU:HD23	2:A:1000:R18:H11A	1.96	0.47
1:A:781:ASP:OD1	1:A:781:ASP:N	2.45	0.47
1:A:897:GLN:HB2	1:A:901:LEU:CD1	2.44	0.47
1:A:700:TYR:CD1	1:A:700:TYR:N	2.83	0.47
1:A:786:GLU:OE2	1:A:802:TRP:CH2	2.67	0.47
1:A:804:ILE:HG12	1:A:880:LEU:CD2	2.44	0.47
1:B:835:LEU:HB2	1:B:838:GLN:HE21	1.80	0.47
1:B:800:THR:HA	1:B:803:GLN:HE21	1.76	0.47
1:B:767:SER:HG	1:B:777:TYR:H	1.52	0.47
1:B:880:LEU:HD23	1:B:883:LEU:HD13	1.96	0.47
2:A:1000:R18:H182	2:A:1000:R18:H8	1.69	0.46
1:B:855:ALA:CA	1:B:858:LEU:HD12	2.40	0.46
1:B:743:HIS:ND1	1:B:745:ASP:HB2	2.30	0.46
1:A:804:ILE:HD13	1:A:804:ILE:HG21	1.76	0.46
1:A:717:SER:O	1:A:718:LEU:C	2.54	0.46
1:A:751:ILE:O	1:A:752:GLN:C	2.54	0.46
1:B:755:TRP:CZ3	1:B:909:MET:HE3	2.50	0.46
1:B:850:ARG:O	1:B:854:LYS:HG3	2.16	0.46
1:A:746:ASP:O	1:A:750:LEU:HG	2.15	0.46
1:A:901:LEU:O	1:A:902:SER:CB	2.61	0.46
1:B:844:MET:CE	1:B:848:TYR:HE2	2.28	0.45
1:B:892:LEU:CD1	1:B:896:ILE:HD11	2.46	0.45
1:B:746:ASP:HB3	1:B:835:LEU:HD22	1.95	0.45
1:B:690:LEU:HD23	1:B:737:PRO:CG	2.40	0.45
1:A:705:ASN:O	1:A:706:THR:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:TYR:CE2	1:B:799:LEU:HD11	2.52	0.45
1:B:780:PRO:HD2	1:B:781:ASP:H	1.82	0.45
1:B:917:LEU:H	1:B:918:PRO:CD	2.24	0.45
1:A:860:GLN:HE21	1:A:860:GLN:CA	2.28	0.45
1:B:739:PHE:CZ	1:B:747:GLN:HA	2.52	0.45
1:A:752:GLN:HE21	1:A:912:VAL:HG12	1.82	0.45
1:B:703:HIS:CG	1:B:704:ASP:N	2.85	0.45
1:B:755:TRP:O	1:B:756:MET:C	2.56	0.45
1:B:837:SER:OG	1:B:840:GLN:NE2	2.49	0.45
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.76	0.45
1:B:779:ALA:HB1	1:B:780:PRO:HD3	1.99	0.45
1:A:765:TRP:CB	1:A:818:PHE:CE1	2.99	0.45
1:A:919:LYS:HD2	1:A:924:MET:O	2.16	0.45
1:B:859:ARG:O	1:B:861:LYS:N	2.47	0.45
1:B:746:ASP:OD1	1:B:835:LEU:HD22	2.16	0.44
1:B:788:ARG:O	1:B:792:SER:HB3	2.17	0.44
1:A:790:LYS:O	1:A:792:SER:N	2.51	0.44
1:B:848:TYR:O	1:B:849:ILE:C	2.56	0.44
1:A:755:TRP:CD1	1:A:755:TRP:N	2.85	0.44
1:A:897:GLN:O	1:A:901:LEU:HG	2.17	0.44
1:B:797:LEU:HD23	1:B:801:MET:HE1	1.98	0.44
1:B:739:PHE:CE2	1:B:747:GLN:HB3	2.53	0.44
1:B:817:GLU:OE2	1:B:856:ILE:HA	2.17	0.44
1:B:828:ASN:HD22	1:B:828:ASN:HA	1.34	0.44
1:A:755:TRP:CZ3	1:A:909:MET:HE2	2.53	0.44
1:A:860:GLN:HG2	1:A:869:ARG:HG2	1.99	0.44
1:B:827:LEU:HD11	1:B:844:MET:HG2	2.00	0.44
1:A:690:LEU:HD23	1:A:694:ILE:HG12	1.99	0.43
1:A:723:GLU:OE1	1:A:909:MET:HB2	2.17	0.43
1:A:743:HIS:O	1:A:746:ASP:HB2	2.18	0.43
1:A:837:SER:O	1:A:838:GLN:C	2.57	0.43
1:B:723:GLU:OE2	1:B:908:MET:HB2	2.17	0.43
1:B:841:PHE:CD1	1:B:841:PHE:C	2.91	0.43
1:B:850:ARG:HA	1:B:853:ILE:HD12	2.00	0.43
1:A:778:PHE:HZ	1:A:801:MET:CE	2.30	0.43
1:A:905:PHE:N	1:A:905:PHE:CD1	2.86	0.43
1:B:720:GLN:HG2	1:B:724:ARG:HH21	1.82	0.43
1:A:889:LEU:O	1:A:889:LEU:HD12	2.17	0.43
1:B:752:GLN:O	1:B:755:TRP:CD1	2.71	0.43
1:B:860:GLN:HB3	1:B:865:SER:OG	2.19	0.43
1:A:720:GLN:CG	1:A:724:ARG:HE	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ASN:O	1:B:720:GLN:C	2.56	0.43
1:B:760:VAL:HG21	1:B:887:LEU:HD11	2.00	0.43
1:B:723:GLU:OE2	1:B:908:MET:HE2	2.19	0.43
1:B:913:ILE:HG12	1:B:917:LEU:HD22	2.01	0.43
1:A:743:HIS:CG	1:A:836:ARG:HD3	2.54	0.42
1:B:719:ASN:ND2	1:B:905:PHE:HA	2.34	0.42
1:A:736:LEU:HA	1:A:737:PRO:HD3	1.78	0.42
1:A:888:HIS:HB3	1:A:921:LEU:HD21	2.00	0.42
1:B:844:MET:HE3	1:B:848:TYR:HE2	1.84	0.42
1:B:871:TYR:CD1	1:B:931:HIS:NE2	2.87	0.42
1:B:706:THR:O	1:B:707:LYS:C	2.58	0.42
1:B:691:LEU:O	1:B:692:MET:C	2.56	0.42
1:A:743:HIS:CE1	1:A:836:ARG:HD3	2.55	0.42
1:B:747:GLN:O	1:B:751:ILE:HD12	2.19	0.42
1:B:917:LEU:HD12	1:B:917:LEU:HA	1.69	0.41
1:A:714:LEU:HD12	1:A:714:LEU:HA	1.80	0.41
1:A:886:GLN:O	1:A:887:LEU:C	2.57	0.41
1:A:799:LEU:O	1:A:802:TRP:CB	2.68	0.41
1:B:800:THR:O	1:B:803:GLN:HB2	2.20	0.41
1:A:744:ILE:HD13	1:A:744:ILE:HA	1.69	0.41
1:B:743:HIS:NE2	1:B:836:ARG:NH1	2.68	0.41
1:A:688:ILE:HG21	1:A:816:GLU:HG3	2.03	0.41
1:A:721:LEU:HD23	2:A:1000:R18:C1	2.51	0.41
1:B:687:LEU:O	1:B:688:ILE:C	2.57	0.41
1:A:703:HIS:HD2	1:A:717:SER:OG	2.03	0.41
1:A:701:ALA:CA	1:A:721:LEU:HD13	2.50	0.41
1:B:777:TYR:OH	1:B:780:PRO:HA	2.20	0.41
1:A:761:PHE:CD2	1:A:822:LYS:HB2	2.55	0.41
1:A:891:CYS:HB2	2:A:1000:R18:H161	2.01	0.41
1:B:750:LEU:HD21	1:B:830:ILE:CG2	2.50	0.41
1:B:752:GLN:O	1:B:755:TRP:HD1	2.03	0.41
1:B:811:LEU:HD23	1:B:811:LEU:HA	1.89	0.41
1:B:869:ARG:HA	1:B:872:GLN:OE1	2.21	0.41
1:A:762:GLY:HA2	1:A:765:TRP:HB3	2.03	0.41
1:A:743:HIS:O	1:A:744:ILE:C	2.59	0.40
1:B:723:GLU:HB2	1:B:906:PRO:HG2	2.03	0.40
1:A:899:ARG:HD2	1:A:899:ARG:HA	1.70	0.40
1:B:695:GLU:HA	1:B:696:PRO:HD3	1.90	0.40
1:A:748:ILE:HG22	1:A:752:GLN:OE1	2.21	0.40
1:A:698:VAL:HG22	1:A:700:TYR:CE1	2.56	0.40
1:A:700:TYR:HD1	1:A:700:TYR:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:PRO:O	1:A:709:ASP:C	2.59	0.40
1:A:750:LEU:HG	1:A:750:LEU:H	1.76	0.40
1:A:752:GLN:O	1:A:755:TRP:CD1	2.73	0.40
1:B:789:MET:O	1:B:791:GLU:N	2.54	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	249/258 (96%)	205 (82%)	30 (12%)	14 (6%)	2 5
1	B	247/258 (96%)	197 (80%)	37 (15%)	13 (5%)	2 6
All	All	496/516 (96%)	402 (81%)	67 (14%)	27 (5%)	2 5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	THR
1	A	787	GLN
1	A	788	ARG
1	A	793	SER
1	B	787	GLN
1	B	789	MET
1	B	790	LYS
1	B	907	GLU
1	A	792	SER
1	A	895	PHE
1	B	788	ARG
1	A	705	ASN
1	B	793	SER
1	A	857	GLY

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Mol	Chain	Res	Type
1	A	896	ILE
1	B	705	ASN
1	B	860	GLN
1	A	764	GLY
1	B	684	ILE
1	B	720	GLN
1	A	863	VAL
1	A	881	HIS
1	B	863	VAL
1	B	882	ASP
1	A	744	ILE
1	B	918	PRO
1	A	918	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	227/240 (95%)	178 (78%)	49 (22%)	1 3
1	B	232/240 (97%)	189 (82%)	43 (18%)	1 5
All	All	459/480 (96%)	367 (80%)	92 (20%)	1 4

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	A	700	TYR
1	A	710	THR
1	A	713	SER
1	A	714	LEU
1	A	715	LEU
1	A	717	SER
1	A	724	ARG
1	A	728	SER
1	A	731	LYS

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Mol	Chain	Res	Type
1	A	733	SER
1	A	737	PRO
1	A	741	ASN
1	A	742	LEU
1	A	744	ILE
1	A	759	MET
1	A	760	VAL
1	A	770	HIS
1	A	774	GLN
1	A	786	GLU
1	A	787	GLN
1	A	789	MET
1	A	799	LEU
1	A	802	TRP
1	A	810	LYS
1	A	821	MET
1	A	822	LYS
1	A	837	SER
1	A	840	GLN
1	A	844	MET
1	A	846	SER
1	A	847	SER
1	A	851	GLU
1	A	854	LYS
1	A	860	GLN
1	A	863	VAL
1	A	864	VAL
1	A	867	SER
1	A	869	ARG
1	A	880	LEU
1	A	897	GLN
1	A	898	SER
1	A	902	SER
1	A	904	GLU
1	A	905	PHE
1	A	909	MET
1	A	917	LEU
1	A	924	MET
1	A	932	LYS
1	B	686	PRO
1	B	697	ASP
1	B	698	VAL

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Mol	Chain	Res	Type
1	B	707	LYS
1	B	713	SER
1	B	720	GLN
1	B	726	LEU
1	B	728	SER
1	B	731	LYS
1	B	734	LYS
1	B	744	ILE
1	B	757	SER
1	B	760	VAL
1	B	766	ARG
1	B	769	LYS
1	B	772	SER
1	B	784	LEU
1	B	788	ARG
1	B	790	LYS
1	B	802	TRP
1	B	804	ILE
1	B	815	GLN
1	B	821	MET
1	B	828	ASN
1	B	830	ILE
1	B	832	LEU
1	B	833	GLU
1	B	839	THR
1	B	845	ARG
1	B	864	VAL
1	B	867	SER
1	B	880	LEU
1	B	882	ASP
1	B	883	LEU
1	B	889	LEU
1	B	892	LEU
1	B	893	ASN
1	B	901	LEU
1	B	908	MET
1	B	909	MET
1	B	910	SER
1	B	911	GLU
1	B	919	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	703	HIS
1	A	720	GLN
1	A	741	ASN
1	A	747	GLN
1	A	828	ASN
1	A	838	GLN
1	A	860	GLN
1	A	868	GLN
1	B	703	HIS
1	B	725	GLN
1	B	752	GLN
1	B	803	GLN
1	B	812	GLN
1	B	815	GLN
1	B	828	ASN
1	B	838	GLN
1	B	840	GLN
1	B	879	ASN
1	B	888	HIS
1	B	893	ASN
1	B	916	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	R18	A	1000	-	21,24,24	1.58	4 (19%)	26,39,39	2.14	10 (38%)
2	R18	B	1000	-	21,24,24	1.28	2 (9%)	26,39,39	2.98	15 (57%)

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	R18	A	1000	-	-	-	0/4/4/4
2	R18	B	1000	-	-	-	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	R18	C11-C9	4.30	1.55	1.44
2	A	1000	R18	C27-C17	3.22	1.57	1.52
2	B	1000	R18	C27-C17	3.17	1.57	1.52
2	B	1000	R18	O83-C3	-2.64	1.18	1.23
2	A	1000	R18	C18-C13	2.08	1.57	1.53
2	A	1000	R18	O97-C17	-2.07	1.41	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	R18	O97-C17-C16	5.16	122.28	109.47
2	B	1000	R18	C14-C8-C9	-5.02	100.84	108.56
2	B	1000	R18	O97-C17-C27	-4.94	97.71	107.66
2	B	1000	R18	O83-C3-C4	-4.84	112.38	121.68
2	A	1000	R18	C7-C6-C5	-4.46	101.20	111.07
2	A	1000	R18	C6-C7-C8	-4.36	102.66	111.46
2	B	1000	R18	C18-C13-C17	-4.23	100.99	111.96
2	A	1000	R18	C27-C17-C16	4.18	118.56	112.24
2	B	1000	R18	C7-C6-C5	-3.95	102.34	111.07
2	B	1000	R18	O83-C3-C2	3.90	129.62	121.57
2	A	1000	R18	C4-C5-C10	-3.22	118.71	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	R18	C8-C9-C11	3.20	119.95	116.54
2	B	1000	R18	C13-C12-C11	-3.13	115.93	122.54
2	B	1000	R18	C1-C2-C3	-3.10	107.14	113.27
2	B	1000	R18	C15-C16-C17	-3.05	104.16	107.22
2	B	1000	R18	C7-C8-C14	-3.00	106.80	111.48
2	B	1000	R18	C4-C5-C10	-2.79	119.13	121.88
2	A	1000	R18	C2-C3-C4	-2.66	112.64	116.74
2	A	1000	R18	C2-C1-C10	-2.45	107.15	112.60
2	B	1000	R18	C14-C13-C12	2.31	109.78	108.18
2	A	1000	R18	C1-C2-C3	-2.22	108.87	113.27
2	A	1000	R18	C7-C8-C14	-2.21	108.03	111.48
2	B	1000	R18	C15-C14-C13	-2.18	102.03	103.40
2	A	1000	R18	O97-C17-C27	-2.12	103.38	107.66
2	A	1000	R18	O83-C3-C2	2.05	125.81	121.57

There are no chirality outliers.

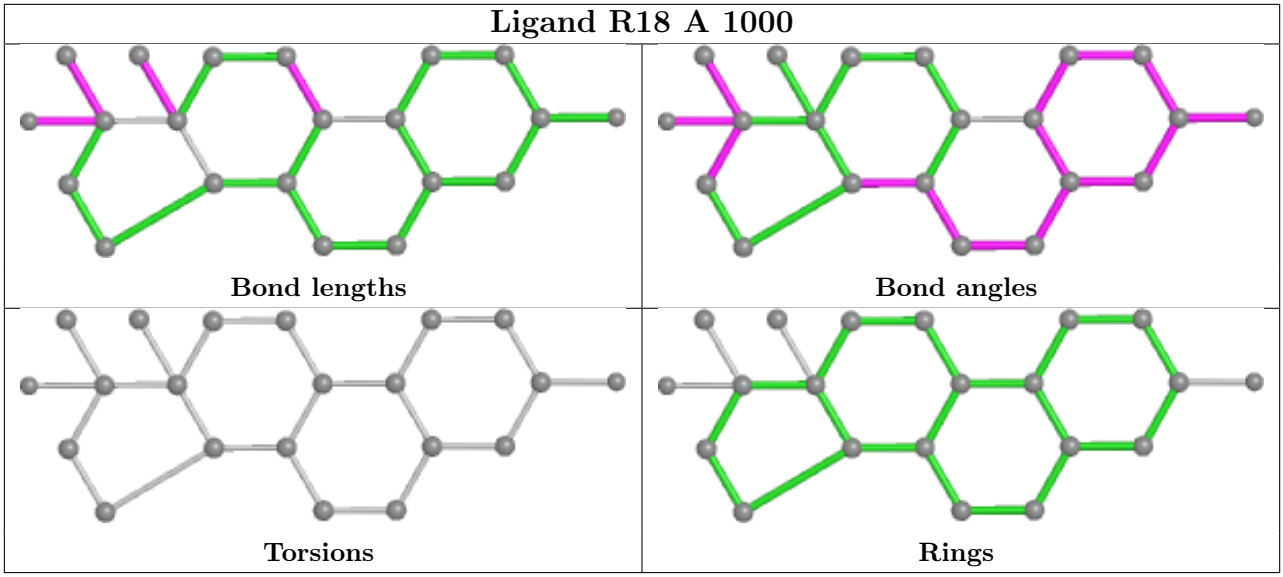
There are no torsion outliers.

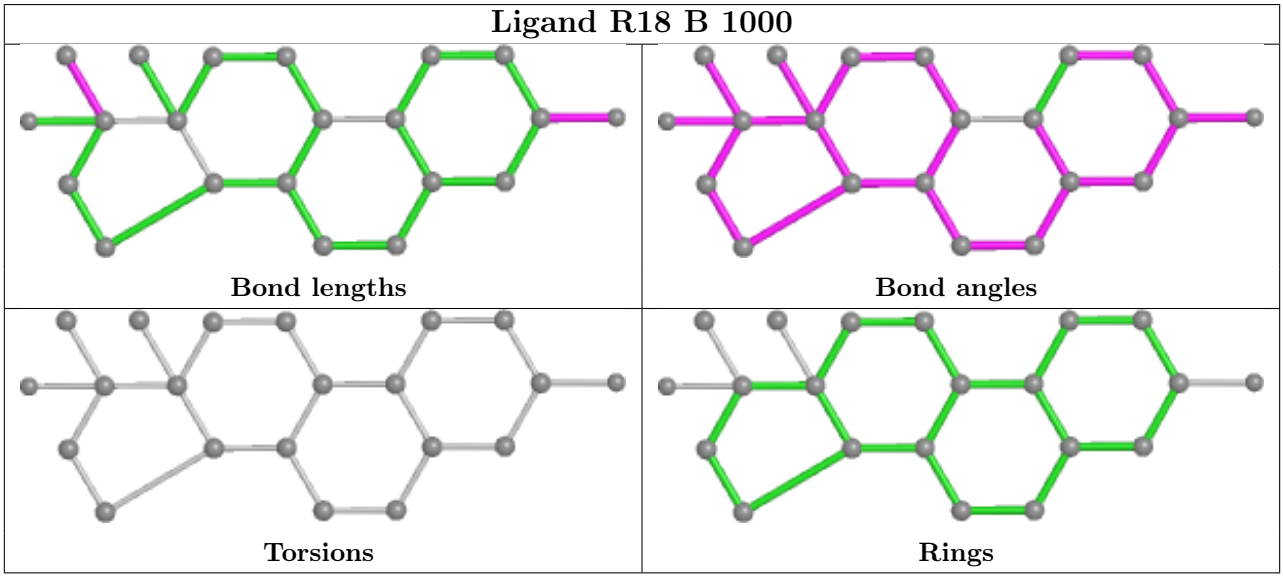
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	R18	5	0
2	B	1000	R18	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	251/258 (97%)	-0.70	1 (0%)	92	91	6, 29, 68, 85	0
1	B	249/258 (96%)	-0.72	2 (0%)	86	81	6, 29, 68, 86	0
All	All	500/516 (96%)	-0.71	3 (0%)	89	86	6, 29, 70, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	ASN	2.9
1	B	708	PRO	2.6
1	B	705	ASN	2.2

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

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

6.3 Carbohydrates (i)

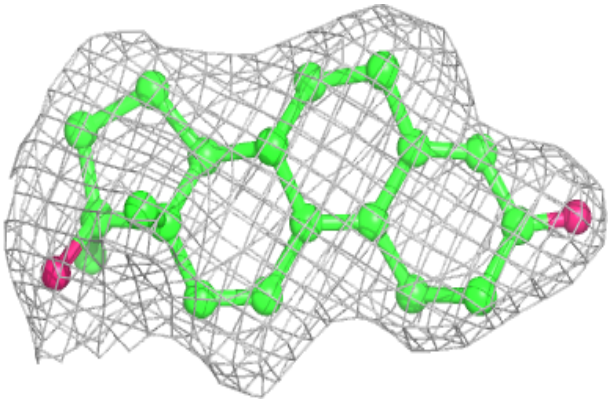
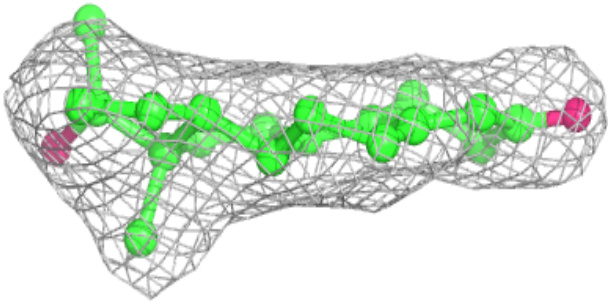
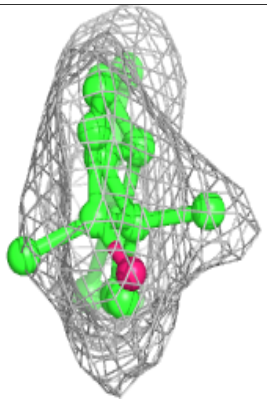
There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

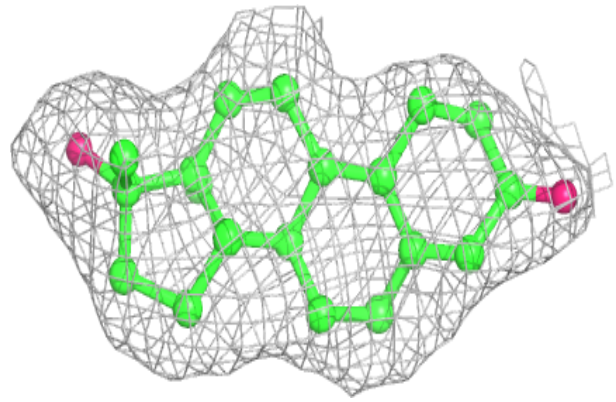
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	R18	B	1000	21/21	0.95	0.12	2,13,19,21	0
2	R18	A	1000	21/21	0.97	0.11	2,5,9,10	0

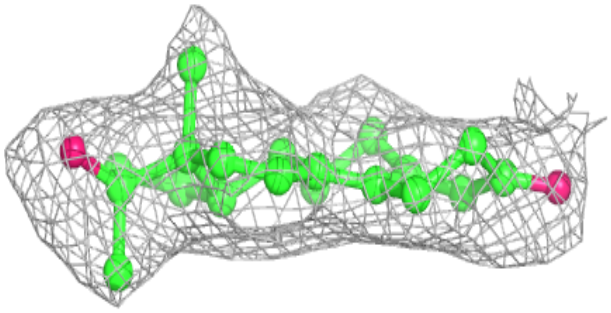
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

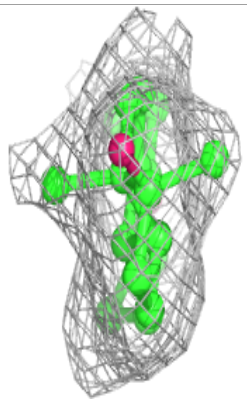
Electron density around R18 B 1000: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around R18 A 1000:

$2mF_o$-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.