



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:56 pm BST

PDB ID : 3SKG
Title : Crystal structure of beta-site app-cleaving enzyme 1 (BACE-WT) complex with (2S)-2-((3R)-3-acetamido-3-isobutyl-2-oxo-1-pyrrolidiny1)-N-((1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-2-(1,2,3,4-tetrahydro-3-isoquinoliny1)ethyl)-4-phenylbutanamide
Authors : Muckelbauer, J.K.
Deposited on : 2011-06-22
Resolution : 2.88 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

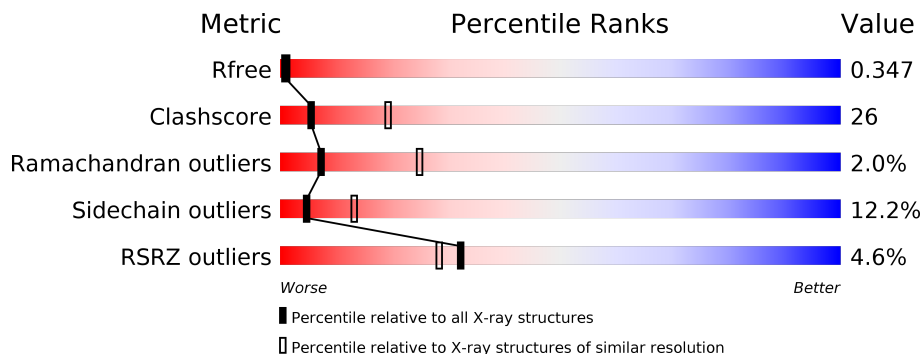
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 on 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	455	 3% 44% 35% 6% 15%
1	B	455	 2% 46% 33% 5% 15%
1	D	455	 5% 36% 41% 6% 15%
1	E	455	 5% 43% 34% 8% 15%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12434 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3034	1944	503	573	14	0	0	0
1	B	386	3034	1944	503	573	14	0	0	0
1	D	386	3034	1944	503	573	14	0	0	0
1	E	386	3034	1944	503	573	14	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

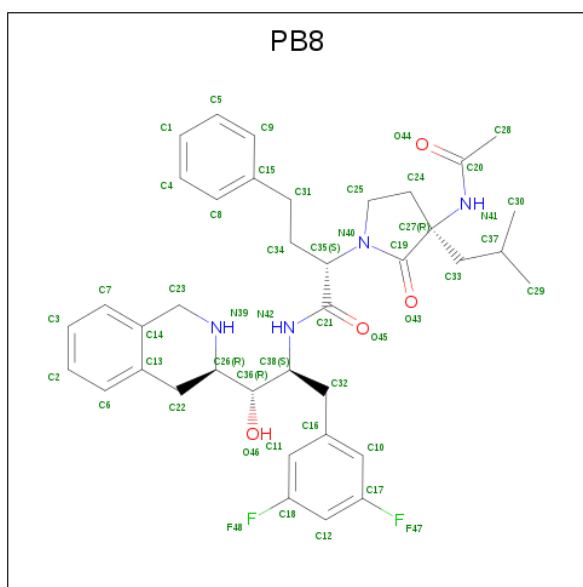
Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	EXPRESSION TAG	UNP P56817
A	-60	ALA	-	EXPRESSION TAG	UNP P56817
A	-59	SER	-	EXPRESSION TAG	UNP P56817
A	-58	MET	-	EXPRESSION TAG	UNP P56817
A	-57	THR	-	EXPRESSION TAG	UNP P56817
A	-56	GLY	-	EXPRESSION TAG	UNP P56817
A	-55	GLY	-	EXPRESSION TAG	UNP P56817
A	-54	GLN	-	EXPRESSION TAG	UNP P56817
A	-53	GLN	-	EXPRESSION TAG	UNP P56817
A	-52	MET	-	EXPRESSION TAG	UNP P56817
A	-51	GLY	-	EXPRESSION TAG	UNP P56817
A	-50	ARG	-	EXPRESSION TAG	UNP P56817
A	-49	GLY	-	EXPRESSION TAG	UNP P56817
A	-48	SER	-	EXPRESSION TAG	UNP P56817
B	-61	MET	-	EXPRESSION TAG	UNP P56817
B	-60	ALA	-	EXPRESSION TAG	UNP P56817
B	-59	SER	-	EXPRESSION TAG	UNP P56817
B	-58	MET	-	EXPRESSION TAG	UNP P56817
B	-57	THR	-	EXPRESSION TAG	UNP P56817
B	-56	GLY	-	EXPRESSION TAG	UNP P56817
B	-55	GLY	-	EXPRESSION TAG	UNP P56817

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-54	GLN	-	EXPRESSION TAG	UNP P56817
B	-53	GLN	-	EXPRESSION TAG	UNP P56817
B	-52	MET	-	EXPRESSION TAG	UNP P56817
B	-51	GLY	-	EXPRESSION TAG	UNP P56817
B	-50	ARG	-	EXPRESSION TAG	UNP P56817
B	-49	GLY	-	EXPRESSION TAG	UNP P56817
B	-48	SER	-	EXPRESSION TAG	UNP P56817
D	-61	MET	-	EXPRESSION TAG	UNP P56817
D	-60	ALA	-	EXPRESSION TAG	UNP P56817
D	-59	SER	-	EXPRESSION TAG	UNP P56817
D	-58	MET	-	EXPRESSION TAG	UNP P56817
D	-57	THR	-	EXPRESSION TAG	UNP P56817
D	-56	GLY	-	EXPRESSION TAG	UNP P56817
D	-55	GLY	-	EXPRESSION TAG	UNP P56817
D	-54	GLN	-	EXPRESSION TAG	UNP P56817
D	-53	GLN	-	EXPRESSION TAG	UNP P56817
D	-52	MET	-	EXPRESSION TAG	UNP P56817
D	-51	GLY	-	EXPRESSION TAG	UNP P56817
D	-50	ARG	-	EXPRESSION TAG	UNP P56817
D	-49	GLY	-	EXPRESSION TAG	UNP P56817
D	-48	SER	-	EXPRESSION TAG	UNP P56817
E	-61	MET	-	EXPRESSION TAG	UNP P56817
E	-60	ALA	-	EXPRESSION TAG	UNP P56817
E	-59	SER	-	EXPRESSION TAG	UNP P56817
E	-58	MET	-	EXPRESSION TAG	UNP P56817
E	-57	THR	-	EXPRESSION TAG	UNP P56817
E	-56	GLY	-	EXPRESSION TAG	UNP P56817
E	-55	GLY	-	EXPRESSION TAG	UNP P56817
E	-54	GLN	-	EXPRESSION TAG	UNP P56817
E	-53	GLN	-	EXPRESSION TAG	UNP P56817
E	-52	MET	-	EXPRESSION TAG	UNP P56817
E	-51	GLY	-	EXPRESSION TAG	UNP P56817
E	-50	ARG	-	EXPRESSION TAG	UNP P56817
E	-49	GLY	-	EXPRESSION TAG	UNP P56817
E	-48	SER	-	EXPRESSION TAG	UNP P56817

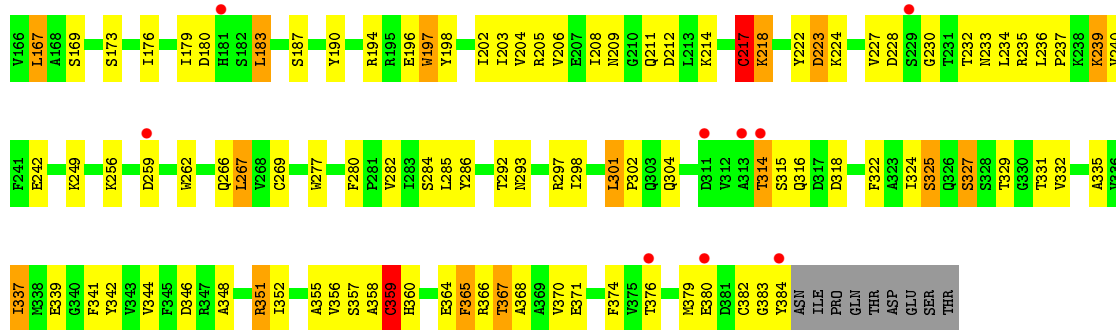
- Molecule 2 is (2S)-2-[(3R)-3-(acetylamino)-3-(2-methylpropyl)-2-oxopyrrolidin-1-yl]-N-[(1R,2S)-3-(3,5-difluorophenyl)-1-hydroxy-1-[(3R)-1,2,3,4-tetrahydroisoquinolin-3-yl]propan-2-yl]-4-phenylbutanamide (three-letter code: PB8) (formula: C₃₈H₄₆F₂N₄O₄).



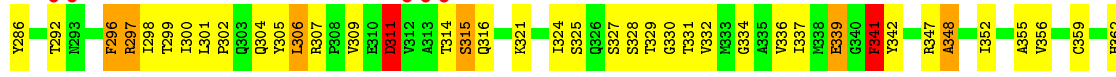
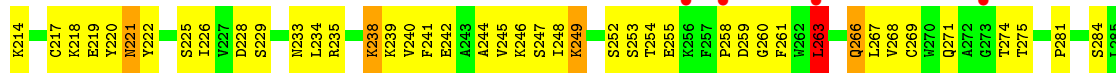
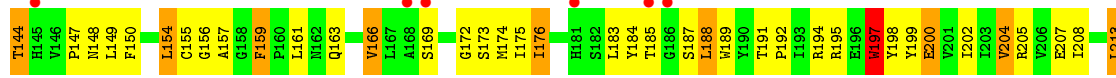
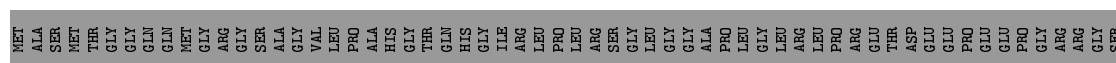
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	A	1	48	38	2	4	4	0	0
2	B	1	48	38	2	4	4	0	0
2	D	1	48	38	2	4	4	0	0
2	E	1	48	38	2	4	4	0	0

- Molecule 3 is water.

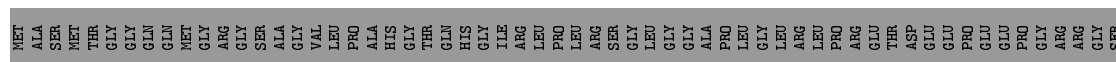
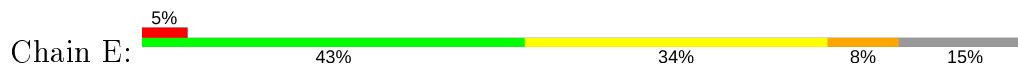
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
3	B	38	38	38	0	0
3	D	20	20	20	0	0
3	E	24	24	24	0	0

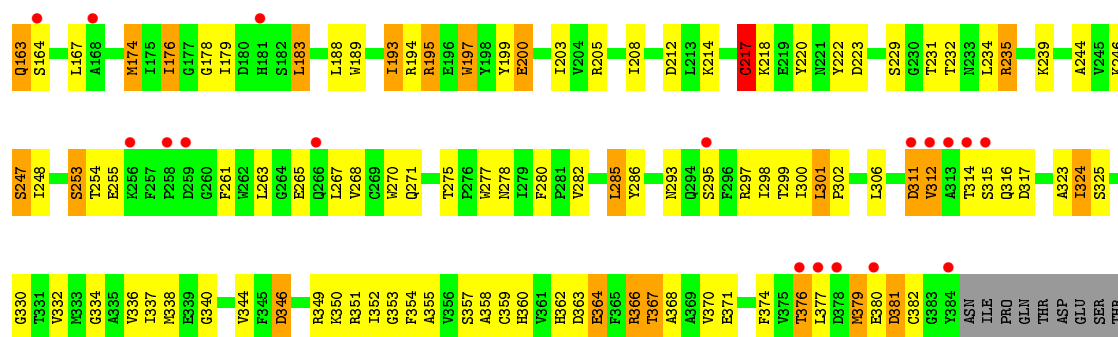


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.24Å 130.45Å 86.87Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	30.63 – 2.88 30.63 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.63-2.88) 98.9 (30.63-2.88)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.255 , 0.348 0.256 , 0.347	Depositor DCC
R_{free} test set	2159 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for l,-k,h	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9537e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PB8

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	1.37	7/3112 (0.2%)	1.21	10/4232 (0.2%)
1	B	1.39	12/3112 (0.4%)	1.24	15/4232 (0.4%)
1	D	1.38	8/3112 (0.3%)	1.22	11/4232 (0.3%)
1	E	1.39	7/3112 (0.2%)	1.26	21/4232 (0.5%)
All	All	1.38	34/12448 (0.3%)	1.23	57/16928 (0.3%)

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	D	0	1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	CYS	CB-SG	-14.77	1.57	1.82
1	E	217	CYS	CB-SG	-11.38	1.62	1.82
1	B	359	CYS	CB-SG	-11.33	1.62	1.82
1	B	364	GLU	CG-CD	9.12	1.65	1.51
1	A	364	GLU	CG-CD	9.08	1.65	1.51
1	A	190	TYR	CD2-CE2	8.21	1.51	1.39
1	B	217	CYS	CB-SG	-8.15	1.68	1.82
1	E	364	GLU	CG-CD	7.48	1.63	1.51
1	B	196	GLU	CG-CD	-6.93	1.41	1.51
1	B	364	GLU	CD-OE2	6.91	1.33	1.25
1	A	217	CYS	CB-SG	-6.53	1.71	1.82
1	B	93	VAL	CB-CG2	6.47	1.66	1.52
1	E	62	ASP	CB-CG	6.26	1.64	1.51
1	B	344	VAL	CB-CG2	-6.23	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	200	GLU	CD-OE1	6.16	1.32	1.25
1	E	311	ASP	CB-CG	6.02	1.64	1.51
1	E	14	TYR	CE1-CZ	6.01	1.46	1.38
1	D	339	GLU	CB-CG	5.77	1.63	1.52
1	D	269	CYS	CB-SG	-5.73	1.72	1.81
1	D	137	PHE	CD2-CE2	5.65	1.50	1.39
1	B	242	GLU	CD-OE1	5.58	1.31	1.25
1	D	348	ALA	CA-CB	5.46	1.64	1.52
1	B	12	GLN	CG-CD	5.46	1.63	1.51
1	B	142	LYS	CD-CE	5.32	1.64	1.51
1	D	155	CYS	CB-SG	5.29	1.91	1.82
1	B	227	VAL	CA-CB	-5.25	1.43	1.54
1	E	79	GLU	CB-CG	5.22	1.62	1.52
1	A	40	VAL	CB-CG2	-5.18	1.42	1.52
1	D	341	PHE	CB-CG	-5.17	1.42	1.51
1	D	4	ASP	CB-CG	5.14	1.62	1.51
1	A	233	ASN	CB-CG	-5.07	1.39	1.51
1	A	341	PHE	CE2-CZ	5.07	1.47	1.37
1	B	365	PHE	CE1-CZ	5.04	1.47	1.37
1	E	364	GLU	CD-OE2	5.01	1.31	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	CYS	CA-CB-SG	-10.02	95.96	114.00
1	E	235	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	B	96	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	E	235	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	E	217	CYS	CA-CB-SG	-8.92	97.95	114.00
1	B	318	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	212	ASP	CB-CG-OD1	8.69	126.12	118.30
1	E	349	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	E	62	ASP	CB-CG-OD1	8.12	125.61	118.30
1	E	64	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	359	CYS	CA-CB-SG	-7.62	100.28	114.00
1	D	131	ASP	CB-CG-OD2	7.56	125.10	118.30
1	D	297	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	4	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	96	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	96	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	63	LEU	CA-CB-CG	6.83	131.00	115.30
1	D	154	LEU	CB-CG-CD1	6.81	122.58	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	D	306	LEU	CB-CG-CD1	-6.64	99.70	111.00
1	E	40	VAL	CB-CA-C	-6.40	99.23	111.40
1	E	138	ASP	CB-CG-OD2	-6.39	112.54	118.30
1	B	227	VAL	CB-CA-C	-6.38	99.27	111.40
1	A	167	LEU	CA-CB-CG	6.36	129.93	115.30
1	B	267	LEU	CA-CB-CG	6.30	129.79	115.30
1	D	377	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	96	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	7	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	84	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	D	83	ASP	CB-CG-OD1	-6.00	112.91	118.30
1	B	83	ASP	CB-CG-OD1	5.96	123.66	118.30
1	E	377	LEU	CA-CB-CG	5.94	128.97	115.30
1	E	349	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	E	311	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	346	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	119	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	D	263	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	4	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	83	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	4	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	231	THR	CA-CB-CG2	-5.59	104.58	112.40
1	B	359	CYS	CA-CB-SG	-5.47	104.16	114.00
1	B	149	LEU	CB-CG-CD1	-5.46	101.71	111.00
1	A	62	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	178	GLY	N-CA-C	5.39	126.58	113.10
1	B	56	LEU	CA-CB-CG	5.34	127.59	115.30
1	D	311	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	119	LEU	CA-CB-CG	5.23	127.34	115.30
1	E	366	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	B	351	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	E	174	MET	CB-CG-SD	5.22	128.06	112.40
1	D	7	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	152	LEU	CA-CB-CG	5.04	126.88	115.30
1	D	161	LEU	CA-CB-CG	5.03	126.88	115.30
1	E	96	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	E	285	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	B	183	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	197	TRP	Peptide

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	3034	0	2948	147	0
1	B	3034	0	2948	127	0
1	D	3034	0	2950	188	0
1	E	3034	0	2948	156	0
2	A	48	0	46	9	0
2	B	48	0	46	7	0
2	D	48	0	46	5	0
2	E	48	0	46	10	0
3	A	24	0	0	7	0
3	B	38	0	0	2	0
3	D	20	0	0	2	0
3	E	24	0	0	3	0
All	All	12434	0	11978	629	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 26.

All (629) 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:73:GLN:HG2	3:A:414:HOH:O	1.43	1.18
1:D:376:THR:HA	3:D:412:HOH:O	1.53	1.07
1:E:63:LEU:HD12	1:E:80:LEU:HB3	1.34	1.07
2:E:394:PB8:H28A	2:E:394:PB8:H31A	1.30	1.07
2:E:394:PB8:H28A	2:E:394:PB8:C31	1.88	1.01
1:A:250:ALA:O	1:A:253:SER:HB2	1.65	0.95
1:B:130:ASP:OD1	1:B:132:SER:HB2	1.67	0.94
1:B:153:GLN:HG2	1:B:183:LEU:HD22	1.47	0.94
1:D:128:ARG:HG2	1:D:128:ARG:HH11	1.34	0.92
1:D:238:LYS:O	1:D:242:GLU:CG	2.19	0.91
1:A:228:ASP:OD2	2:A:394:PB8:N39	2.03	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:MET:HE3	1:B:87:ILE:HG12	1.53	0.90
1:B:359:CYS:HB3	3:B:420:HOH:O	1.71	0.89
1:D:128:ARG:CG	1:D:128:ARG:HH11	1.85	0.89
1:A:241:PHE:CD2	1:A:326:GLN:HG3	2.09	0.88
1:B:234:LEU:HD13	1:B:337:ILE:HD12	1.56	0.88
1:D:238:LYS:O	1:D:242:GLU:HG3	1.76	0.86
1:A:194:ARG:HH12	1:A:384:TYR:H	1.24	0.85
1:D:70:PRO:HD2	1:D:128:ARG:NH2	1.91	0.85
1:D:304:GLN:O	1:D:336:VAL:HB	1.77	0.84
1:B:235:ARG:HB2	1:B:332:VAL:HB	1.59	0.84
1:E:232:THR:O	1:E:336:VAL:HG13	1.78	0.84
1:E:19:THR:OG1	1:E:86:SER:HB2	1.78	0.83
1:E:18:MET:HB2	1:E:29:ILE:CD1	2.08	0.83
2:B:394:PB8:H24	2:B:394:PB8:C28	2.09	0.82
1:E:193:ILE:HG13	1:E:350:LYS:C	2.00	0.82
1:E:18:MET:HB2	1:E:29:ILE:HD13	1.60	0.82
1:E:357:SER:C	1:E:359:CYS:H	1.80	0.82
1:A:315:SER:OG	1:A:316:GLN:N	2.08	0.81
1:D:137:PHE:HE1	1:D:176:ILE:HG23	1.46	0.81
2:B:394:PB8:H24	2:B:394:PB8:H28B	1.63	0.80
1:E:311:ASP:OD2	1:E:315:SER:HB3	1.81	0.80
1:E:18:MET:SD	1:E:29:ILE:HD13	2.21	0.80
1:D:235:ARG:CZ	2:D:394:PB8:H8	2.12	0.79
1:D:45:HIS:CG	1:D:46:PRO:HD2	2.18	0.79
1:D:2:MET:SD	1:D:91:PRO:HD3	2.23	0.78
1:E:30:LEU:HD23	1:E:118:ILE:HD12	1.66	0.78
1:A:194:ARG:NH1	1:A:384:TYR:H	1.79	0.78
1:B:163:GLN:O	1:B:167:LEU:HD12	1.83	0.78
1:A:123:TYR:CE1	1:A:196:GLU:HG2	2.18	0.78
1:D:188:LEU:HD13	1:D:355:ALA:HB2	1.66	0.78
1:E:85:VAL:HG11	1:E:136:PHE:HE1	1.48	0.77
1:D:48:LEU:HD21	1:D:109:PHE:CD1	2.19	0.77
1:D:128:ARG:NH1	1:D:128:ARG:HG2	1.94	0.77
1:E:36:SER:OG	1:E:126:ILE:HG13	1.83	0.77
1:A:20:VAL:O	1:A:25:GLN:HG3	1.85	0.77
1:E:315:SER:OG	1:E:316:GLN:N	2.11	0.76
1:D:17:GLU:O	1:D:88:PRO:HD2	1.86	0.76
1:D:238:LYS:O	1:D:242:GLU:HG2	1.84	0.75
1:A:194:ARG:HH12	1:A:384:TYR:N	1.82	0.75
1:D:10:SER:OG	1:D:307:ARG:HD3	1.86	0.75
1:D:195:ARG:O	1:D:197:TRP:HD1	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:LEU:HD21	1:E:82:THR:HG23	1.67	0.75
1:D:202:ILE:HG21	1:D:382:CYS:SG	2.27	0.74
1:D:6:LEU:HD22	1:D:14:TYR:HB3	1.70	0.74
1:A:222:TYR:O	1:A:330:GLY:HA2	1.88	0.73
1:E:357:SER:OG	1:E:359:CYS:HB3	1.89	0.73
1:D:356:VAL:HG23	3:D:397:HOH:O	1.88	0.72
1:E:20:VAL:O	1:E:25:GLN:HG3	1.88	0.72
1:D:29:ILE:HG23	1:D:118:ILE:N	2.04	0.72
1:D:205:ARG:HA	1:D:220:TYR:HE2	1.55	0.72
1:D:85:VAL:HG11	1:D:136:PHE:CE1	2.24	0.72
1:E:234:LEU:HB2	1:E:337:ILE:HD13	1.71	0.72
1:B:298:ILE:HG22	1:B:370:VAL:HG22	1.72	0.71
1:A:123:TYR:CZ	1:A:196:GLU:HG2	2.25	0.71
1:E:346:ASP:HB3	1:E:351:ARG:HG3	1.73	0.71
2:E:394:PB8:H28B	2:E:394:PB8:H24	1.72	0.71
1:D:2:MET:CE	1:D:91:PRO:HD3	2.21	0.71
1:A:207:GLU:O	1:A:208:ILE:HD13	1.91	0.70
1:A:91:PRO:HD3	1:A:176:ILE:HD13	1.74	0.70
1:A:235:ARG:NH1	1:A:326:GLN:O	2.25	0.70
1:B:249:LYS:HG2	1:B:262:TRP:CZ2	2.26	0.69
1:D:28:ASN:C	1:D:29:ILE:HD13	2.12	0.69
1:E:63:LEU:HG	1:E:81:GLY:HA2	1.75	0.69
1:D:2:MET:HE1	1:D:91:PRO:HD3	1.72	0.69
1:D:194:ARG:HB3	1:D:200:GLU:OE1	1.92	0.69
1:B:322:PHE:CZ	1:B:324:ILE:HD12	2.27	0.69
1:A:357:SER:C	1:A:359:CYS:H	1.95	0.69
1:A:235:ARG:NH2	1:A:327:SER:HB2	2.07	0.69
1:E:234:LEU:HB3	1:E:324:ILE:HG23	1.74	0.69
1:B:267:LEU:HD13	1:B:269:CYS:SG	2.33	0.68
1:E:197:TRP:H	1:E:197:TRP:HD1	1.40	0.68
1:E:189:TRP:O	1:E:353:GLY:HA2	1.93	0.68
1:B:149:LEU:HD12	1:B:346:ASP:HA	1.74	0.68
1:D:188:LEU:CD1	1:D:355:ALA:HB2	2.23	0.68
1:A:2:MET:SD	1:A:90:GLY:HA2	2.34	0.68
1:D:70:PRO:HD2	1:D:128:ARG:HH21	1.56	0.68
1:D:51:TYR:N	1:D:51:TYR:HD2	1.91	0.67
1:E:357:SER:C	1:E:359:CYS:N	2.48	0.67
2:E:394:PB8:H28A	2:E:394:PB8:H31	1.77	0.67
2:E:394:PB8:H31A	2:E:394:PB8:C28	2.18	0.67
1:D:173:SER:HB3	1:D:175:ILE:HD11	1.76	0.67
1:A:221:ASN:ND2	1:A:225:SER:HB2	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:SER:HB3	1:E:344:VAL:HG22	1.77	0.66
1:D:258:PRO:HG2	1:D:266:GLN:OE1	1.96	0.66
1:D:379:MET:O	1:D:381:ASP:N	2.29	0.66
1:B:18:MET:CE	1:B:87:ILE:HG12	2.25	0.66
1:A:22:SER:O	1:A:57:SER:HA	1.96	0.66
1:D:2:MET:HG2	1:D:90:GLY:HA2	1.78	0.66
1:E:263:LEU:HB3	1:E:265:GLU:HG3	1.77	0.66
1:B:50:ARG:O	1:B:116:GLU:HG2	1.96	0.66
1:E:205:ARG:HB3	1:E:286:TYR:HB2	1.78	0.65
1:B:218:LYS:HE2	1:B:383:GLY:O	1.96	0.65
1:D:137:PHE:CE1	1:D:176:ILE:HG23	2.30	0.65
1:D:207:GLU:O	1:D:208:ILE:HD13	1.96	0.65
1:D:70:PRO:CD	1:D:128:ARG:NH2	2.59	0.65
1:E:188:LEU:HD23	1:E:355:ALA:HB2	1.79	0.65
1:A:218:LYS:HE2	1:A:381:ASP:O	1.96	0.65
1:E:140:LEU:HD12	1:E:140:LEU:O	1.96	0.65
1:D:22:SER:HB2	1:D:59:THR:HG22	1.77	0.65
1:E:302:PRO:O	1:E:306:LEU:HB2	1.96	0.65
1:B:233:ASN:HD22	1:B:325:SER:HB3	1.62	0.64
1:B:234:LEU:O	1:B:324:ILE:HA	1.97	0.64
1:A:376:THR:HG22	1:B:365:PHE:HZ	1.63	0.64
1:E:141:VAL:HG13	1:E:146:VAL:O	1.97	0.64
1:E:232:THR:HB	3:E:402:HOH:O	1.97	0.64
1:A:47:PHE:CE1	1:A:111:ASN:HB2	2.33	0.64
1:D:26:THR:O	1:D:27:LEU:HD23	1.98	0.64
1:A:279:ILE:HA	1:B:211:GLN:HG3	1.79	0.63
1:E:21:GLY:O	1:E:24:PRO:HA	1.99	0.63
1:A:67:VAL:HG11	1:A:80:LEU:CD2	2.27	0.63
1:B:234:LEU:HD13	1:B:337:ILE:CD1	2.26	0.63
1:D:296:PHE:CD2	1:D:296:PHE:N	2.66	0.63
1:E:32:ASP:OD1	1:E:34:GLY:N	2.30	0.63
1:D:33:THR:OG1	1:D:228:ASP:HA	1.98	0.63
1:A:208:ILE:HG21	1:A:247:SER:HB3	1.80	0.62
1:D:260:GLY:HA2	1:D:263:LEU:HB2	1.81	0.62
1:A:304:GLN:O	1:A:336:VAL:HB	1.98	0.62
1:B:31:VAL:HG11	1:B:152:LEU:HD21	1.81	0.62
1:E:33:THR:N	1:E:229:SER:OG	2.30	0.62
1:B:140:LEU:O	1:B:144:THR:OG1	2.17	0.62
1:A:239:LYS:CB	1:A:239:LYS:NZ	2.63	0.62
1:D:156:GLY:H	1:D:339:GLU:HG2	1.63	0.62
1:B:163:GLN:O	1:B:167:LEU:CD1	2.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG11	1:A:80:LEU:HD21	1.82	0.62
1:D:51:TYR:N	1:D:51:TYR:CD2	2.67	0.61
1:D:38:PHE:CE2	1:D:99:ILE:HG13	2.36	0.61
1:A:52:TYR:CE2	1:A:54:ARG:HG2	2.35	0.61
1:D:205:ARG:HA	1:D:220:TYR:CE2	2.34	0.60
1:D:315:SER:OG	1:D:316:GLN:N	2.32	0.60
1:D:194:ARG:NH2	1:D:384:TYR:O	2.30	0.60
1:D:85:VAL:HG11	1:D:136:PHE:HE1	1.67	0.60
1:A:149:LEU:O	1:A:177:GLY:HA2	2.02	0.60
1:A:54:ARG:O	1:A:56:LEU:N	2.34	0.60
1:D:22:SER:HB2	1:D:59:THR:CG2	2.31	0.60
1:A:205:ARG:NE	1:A:207:GLU:OE2	2.29	0.60
1:B:346:ASP:HB3	1:B:351:ARG:HG2	1.84	0.60
1:A:47:PHE:CD1	1:A:111:ASN:HB2	2.37	0.59
1:A:318:ASP:OD2	3:A:418:HOH:O	2.16	0.59
1:D:302:PRO:HA	1:D:305:TYR:CE2	2.36	0.59
2:A:394:PB8:H30	2:A:394:PB8:H10	1.85	0.59
1:D:2:MET:HE1	1:D:91:PRO:CD	2.32	0.59
1:D:125:GLU:HG2	1:D:197:TRP:HB3	1.84	0.58
1:B:41:GLY:HA2	1:B:102:ILE:HB	1.85	0.58
1:D:207:GLU:C	1:D:208:ILE:HD13	2.23	0.58
1:B:206:VAL:HG22	1:B:285:LEU:HD23	1.86	0.58
1:E:212:ASP:OD1	1:E:214:LYS:N	2.26	0.58
1:B:206:VAL:HG22	1:B:285:LEU:CD2	2.33	0.58
1:B:32:ASP:OD1	1:B:34:GLY:N	2.34	0.58
1:B:110:ILE:CD1	2:B:394:PB8:H30A	2.33	0.58
1:D:38:PHE:CE2	1:D:99:ILE:CG1	2.87	0.58
1:D:19:THR:OG1	1:D:86:SER:HB3	2.03	0.58
1:A:363:ASP:HB2	1:A:364:GLU:OE2	2.02	0.58
1:D:2:MET:HE2	1:D:176:ILE:H	1.67	0.58
1:D:311:ASP:O	1:D:314:THR:N	2.36	0.58
1:E:193:ILE:HG13	1:E:350:LYS:O	2.04	0.57
1:A:38:PHE:CD1	1:A:119:LEU:HD12	2.40	0.57
1:B:4:ASP:H	1:B:173:SER:HG	1.52	0.57
1:A:148:ASN:O	1:A:347:ARG:HB2	2.04	0.57
1:B:205:ARG:HB3	1:B:286:TYR:CG	2.39	0.57
1:D:110:ILE:O	1:D:113:SER:HB3	2.04	0.57
1:B:110:ILE:HD11	2:B:394:PB8:H30A	1.86	0.57
1:D:10:SER:HG	1:D:307:ARG:HD3	1.69	0.57
1:A:193:ILE:HG22	1:A:195:ARG:H	1.68	0.57
1:B:29:ILE:HD12	1:B:117:GLY:HA3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.40	0.57
1:D:195:ARG:O	1:D:197:TRP:CD1	2.55	0.57
1:D:197:TRP:CD1	1:D:197:TRP:N	2.72	0.57
1:D:204:VAL:HG11	1:D:379:MET:HG2	1.87	0.57
1:D:45:HIS:ND1	1:D:46:PRO:HD2	2.18	0.57
1:E:153:GLN:OE1	1:E:183:LEU:HD22	2.04	0.57
1:B:3:VAL:O	1:B:4:ASP:HB2	2.05	0.57
1:D:140:LEU:HD21	1:D:176:ILE:HG21	1.86	0.57
1:D:188:LEU:HD13	1:D:355:ALA:CB	2.34	0.57
1:B:197:TRP:CG	1:B:198:TYR:N	2.69	0.57
1:A:236:LEU:HD23	1:A:331:THR:HG23	1.86	0.56
1:E:28:ASN:HB2	1:E:116:GLU:OE2	2.04	0.56
1:E:195:ARG:HG2	1:E:197:TRP:CD1	2.40	0.56
1:B:235:ARG:NH1	2:B:394:PB8:H4	2.20	0.56
1:B:357:SER:C	1:B:359:CYS:H	2.09	0.56
1:E:85:VAL:HG11	1:E:136:PHE:CE1	2.35	0.56
1:E:37:ASN:HB2	3:E:400:HOH:O	2.05	0.56
1:E:20:VAL:HB	1:E:85:VAL:HG23	1.88	0.56
1:A:260:GLY:C	1:A:266:GLN:HG2	2.26	0.56
1:A:137:PHE:CZ	1:A:150:PHE:HB3	2.40	0.56
1:A:349:ARG:NH1	3:A:417:HOH:O	2.16	0.56
1:B:45:HIS:HE1	1:B:47:PHE:CD2	2.24	0.56
1:E:346:ASP:CB	1:E:351:ARG:HE	2.18	0.56
1:E:45:HIS:HB3	1:E:48:LEU:HD22	1.88	0.56
1:B:282:VAL:HG13	1:B:366:ARG:NH1	2.21	0.56
1:D:241:PHE:HE1	1:D:324:ILE:HG22	1.70	0.56
1:A:137:PHE:O	1:A:141:VAL:HG23	2.06	0.55
1:E:16:VAL:HG21	1:E:174:MET:CE	2.36	0.55
1:E:253:SER:O	1:E:255:GLU:N	2.40	0.55
1:E:19:THR:HB	1:E:24:PRO:HB2	1.88	0.55
1:B:218:LYS:HA	1:B:382:CYS:O	2.07	0.55
1:E:367:THR:HG23	1:E:368:ALA:O	2.06	0.55
1:D:218:LYS:HE3	1:D:381:ASP:O	2.06	0.55
1:E:286:TYR:CE1	1:E:297:ARG:HD3	2.43	0.54
1:A:234:LEU:HB2	1:A:337:ILE:HD11	1.90	0.54
1:D:217:CYS:SG	1:D:382:CYS:HB3	2.47	0.54
1:E:130:ASP:OD1	1:E:132:SER:HB3	2.07	0.54
2:E:394:PB8:C28	2:E:394:PB8:H24	2.37	0.54
1:B:356:VAL:HG23	1:B:370:VAL:HG23	1.89	0.54
1:D:225:SER:HA	1:D:331:THR:O	2.08	0.54
1:A:194:ARG:NH1	1:A:384:TYR:N	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:TRP:HB2	1:D:102:ILE:HG23	1.90	0.54
1:D:5:ASN:OD1	1:D:173:SER:HA	2.06	0.54
1:E:280:PHE:HB3	1:E:302:PRO:HB3	1.90	0.54
1:A:364:GLU:H	1:A:364:GLU:CD	2.11	0.54
1:B:335:ALA:O	1:B:339:GLU:HG3	2.08	0.54
1:A:189:TRP:HA	3:A:411:HOH:O	2.08	0.53
1:D:286:TYR:OH	1:D:297:ARG:NH1	2.41	0.53
1:B:153:GLN:CG	1:B:183:LEU:HD22	2.30	0.53
1:A:130:ASP:OD2	1:A:132:SER:N	2.36	0.53
1:D:32:ASP:HA	1:D:229:SER:OG	2.08	0.53
1:E:295:SER:HB3	1:E:379:MET:HE1	1.90	0.53
1:A:200:GLU:HA	1:A:225:SER:O	2.08	0.53
1:B:194:ARG:HD2	1:B:202:ILE:HD11	1.90	0.53
1:B:232:THR:HG22	1:B:233:ASN:OD1	2.08	0.53
1:B:34:GLY:O	2:B:394:PB8:N39	2.39	0.53
1:E:357:SER:O	1:E:359:CYS:N	2.41	0.53
1:B:357:SER:OG	1:B:359:CYS:HB2	2.09	0.53
1:A:221:ASN:ND2	1:A:225:SER:CB	2.72	0.53
1:A:15:TYR:CD1	1:A:28:ASN:HB3	2.44	0.53
1:D:226:ILE:HD11	2:D:394:PB8:H23	1.91	0.53
1:D:28:ASN:HB2	1:D:115:TRP:HA	1.92	0.53
1:E:26:THR:HG22	1:E:50:ARG:NH1	2.24	0.53
1:D:298:ILE:HD12	1:D:341:PHE:CE2	2.44	0.52
1:A:346:ASP:OD2	1:A:349:ARG:HD3	2.09	0.52
1:D:121:LEU:HD13	1:D:150:PHE:CE1	2.44	0.52
1:E:188:LEU:CD2	1:E:355:ALA:HB2	2.38	0.52
1:E:32:ASP:C	1:E:34:GLY:H	2.12	0.52
1:A:149:LEU:O	1:A:177:GLY:CA	2.57	0.52
1:B:277:TRP:HE3	1:B:302:PRO:HG2	1.74	0.52
1:D:20:VAL:HG12	1:D:52:TYR:CE1	2.44	0.52
1:D:334:GLY:O	1:D:337:ILE:HB	2.10	0.52
1:E:95:VAL:HG21	1:E:140:LEU:HD13	1.90	0.52
1:A:267:LEU:HD12	1:A:267:LEU:O	2.08	0.52
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.45	0.52
1:D:124:ALA:O	1:D:126:ILE:N	2.43	0.52
1:E:235:ARG:HB2	1:E:332:VAL:HB	1.92	0.52
1:D:110:ILE:HD12	1:D:115:TRP:CZ2	2.45	0.52
1:D:245:VAL:O	1:D:249:LYS:HB2	2.10	0.52
1:D:298:ILE:HG22	1:D:370:VAL:HG22	1.90	0.52
1:D:20:VAL:CG1	1:D:52:TYR:CE1	2.92	0.52
1:D:140:LEU:O	1:D:144:THR:HG22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASP:HA	1:D:229:SER:HG	1.75	0.52
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.92	0.52
1:D:122:ALA:CB	1:D:126:ILE:HD11	2.40	0.52
1:E:197:TRP:N	1:E:197:TRP:CD1	2.76	0.52
1:A:309:VAL:HG21	1:A:321:LYS:HD2	1.92	0.52
1:D:32:ASP:OD1	1:D:34:GLY:N	2.40	0.52
1:D:2:MET:CE	1:D:176:ILE:H	2.23	0.51
1:B:280:PHE:HB2	1:B:302:PRO:HG3	1.92	0.51
1:D:37:ASN:HD21	1:D:128:ARG:H	1.58	0.51
1:A:14:TYR:CG	1:A:154:LEU:HD22	2.45	0.51
1:E:40:VAL:C	1:E:102:ILE:HD12	2.30	0.51
1:A:327:SER:OG	1:A:330:GLY:O	2.16	0.51
1:E:2:MET:HE1	1:E:91:PRO:HD3	1.93	0.51
1:A:77:GLU:HB3	1:A:104:GLU:HB2	1.92	0.51
1:B:18:MET:HG3	1:B:29:ILE:HG12	1.93	0.51
1:E:-1:PHE:HB3	1:E:2:MET:HG3	1.93	0.51
1:E:110:ILE:CD1	2:E:394:PB8:H30	2.41	0.51
1:E:19:THR:CG2	1:E:24:PRO:HB2	2.41	0.51
1:A:149:LEU:HD12	1:A:149:LEU:C	2.31	0.51
1:A:364:GLU:O	1:B:374:PHE:HE1	1.93	0.51
1:B:224:LYS:HE2	3:B:419:HOH:O	2.10	0.51
1:D:234:LEU:O	1:D:324:ILE:HA	2.12	0.51
1:A:121:LEU:CD1	1:A:174:MET:HE2	2.41	0.50
1:A:245:VAL:O	1:A:249:LYS:HB2	2.11	0.50
1:A:54:ARG:C	1:A:56:LEU:N	2.64	0.50
1:D:4:ASP:N	1:D:173:SER:OG	2.22	0.50
1:D:22:SER:O	1:D:57:SER:HA	2.10	0.50
1:A:54:ARG:C	1:A:56:LEU:H	2.15	0.50
1:B:228:ASP:OD1	1:B:230:GLY:N	2.36	0.50
1:D:305:TYR:CD1	1:D:324:ILE:HD12	2.46	0.50
1:E:282:VAL:HG13	1:E:366:ARG:HH11	1.75	0.50
1:A:363:ASP:OD1	1:A:363:ASP:C	2.50	0.50
1:B:126:ILE:HD13	1:B:198:TYR:CE1	2.46	0.50
1:B:69:VAL:HG22	1:B:128:ARG:HB2	1.93	0.50
1:A:83:ASP:OD1	1:A:84:LEU:N	2.43	0.50
1:B:68:TYR:CZ	1:B:70:PRO:HG3	2.45	0.50
1:D:38:PHE:HE2	1:D:99:ILE:CG1	2.23	0.50
1:E:163:GLN:HG2	1:E:167:LEU:HD11	1.93	0.50
1:E:55:GLN:N	1:E:55:GLN:OE1	2.30	0.50
1:A:45:HIS:HB3	1:A:48:LEU:HD12	1.91	0.50
1:D:34:GLY:HA3	2:D:394:PB8:HN39	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:O	1:B:27:LEU:HG	2.12	0.50
1:A:28:ASN:HB2	1:A:115:TRP:HA	1.94	0.50
1:D:219:GLU:OE1	1:D:239:LYS:HE2	2.12	0.50
1:E:124:ALA:O	1:E:125:GLU:C	2.50	0.50
1:A:349:ARG:O	1:A:350:LYS:C	2.47	0.50
1:E:376:THR:O	1:E:379:MET:HE2	2.12	0.49
1:E:63:LEU:HG	1:E:81:GLY:CA	2.40	0.49
1:A:9:LYS:O	1:A:10:SER:C	2.51	0.49
1:A:197:TRP:CG	1:A:198:TYR:N	2.76	0.49
1:A:357:SER:C	1:A:359:CYS:N	2.62	0.49
1:B:130:ASP:OD1	1:B:130:ASP:C	2.51	0.49
1:B:380:GLU:OE1	1:B:380:GLU:N	2.45	0.49
1:D:36:SER:OG	1:D:122:ALA:HB3	2.11	0.49
1:A:121:LEU:CD1	1:A:174:MET:CE	2.90	0.49
1:E:31:VAL:HG22	1:E:119:LEU:HD23	1.95	0.49
1:A:157:ALA:O	1:A:159:PHE:CE2	2.65	0.49
1:A:357:SER:OG	1:A:359:CYS:HB3	2.12	0.49
1:B:45:HIS:CE1	1:B:47:PHE:H	2.30	0.49
1:A:162:ASN:HD22	1:A:165:GLU:H	1.61	0.49
1:D:1:GLU:HG3	1:D:2:MET:HG3	1.95	0.49
1:D:274:THR:O	1:D:275:THR:C	2.49	0.49
1:D:281:PRO:HD2	1:D:305:TYR:OH	2.13	0.49
1:D:261:PHE:HZ	1:D:306:LEU:CD2	2.26	0.49
1:E:253:SER:C	1:E:255:GLU:N	2.65	0.49
1:A:10:SER:OG	1:A:307:ARG:CD	2.60	0.49
1:D:40:VAL:HG12	1:D:117:GLY:HA3	1.95	0.49
1:D:38:PHE:CD2	1:D:99:ILE:HG13	2.48	0.49
1:E:297:ARG:HB2	1:E:374:PHE:CE2	2.47	0.49
1:D:147:PRO:HB2	1:D:149:LEU:HD23	1.95	0.49
1:D:20:VAL:N	1:D:25:GLN:O	2.42	0.49
1:D:4:ASP:H	1:D:173:SER:HG	1.56	0.49
1:E:336:VAL:HG23	1:E:337:ILE:HD12	1.95	0.49
1:E:47:PHE:HB3	1:E:111:ASN:HA	1.95	0.49
1:B:360:HIS:CD2	1:B:368:ALA:HB3	2.48	0.48
1:E:136:PHE:C	1:E:136:PHE:CD2	2.85	0.48
1:E:91:PRO:HB2	1:E:93:VAL:HG22	1.94	0.48
1:B:23:PRO:CB	1:B:24:PRO:HD2	2.43	0.48
1:E:277:TRP:HE3	1:E:302:PRO:HG2	1.76	0.48
1:A:239:LYS:CB	1:A:239:LYS:HZ2	2.26	0.48
1:B:124:ALA:O	1:B:125:GLU:C	2.50	0.48
1:B:237:PRO:HD2	1:B:240:VAL:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:GLN:HE21	1:E:359:CYS:HB2	1.79	0.48
1:E:205:ARG:HA	1:E:220:TYR:CE2	2.49	0.48
1:D:199:TYR:OH	1:D:347:ARG:NH1	2.35	0.48
1:B:239:LYS:CB	1:B:239:LYS:NZ	2.76	0.48
1:D:234:LEU:HD13	1:D:337:ILE:HG13	1.95	0.48
1:A:32:ASP:OD2	2:A:394:PB8:H32A	2.13	0.48
1:D:253:SER:O	1:D:255:GLU:N	2.46	0.48
1:E:218:LYS:HE3	1:E:381:ASP:O	2.14	0.48
1:A:239:LYS:HB3	1:A:239:LYS:NZ	2.28	0.48
1:E:203:ILE:HG23	1:E:286:TYR:O	2.14	0.48
1:E:26:THR:CG2	1:E:27:LEU:N	2.77	0.48
1:B:3:VAL:HG12	1:B:4:ASP:N	2.29	0.47
1:E:29:ILE:HG23	1:E:118:ILE:N	2.29	0.47
1:A:133:LEU:HD23	3:A:401:HOH:O	2.13	0.47
1:A:283:ILE:HD12	1:A:300:ILE:HD11	1.96	0.47
1:D:28:ASN:O	1:D:29:ILE:HD13	2.14	0.47
1:A:261:PHE:N	1:A:266:GLN:HG2	2.29	0.47
1:B:39:ALA:O	1:B:118:ILE:N	2.46	0.47
1:E:74:GLY:HA2	1:E:106:ASP:O	2.13	0.47
1:B:205:ARG:HB3	1:B:286:TYR:CD2	2.49	0.47
1:D:38:PHE:CE2	1:D:99:ILE:HG12	2.48	0.47
1:A:300:ILE:HD12	1:A:305:TYR:HD2	1.80	0.47
1:B:301:LEU:HD21	1:B:367:THR:C	2.34	0.47
2:D:394:PB8:HN41	2:D:394:PB8:H30	1.79	0.47
1:E:334:GLY:O	1:E:338:MET:HG3	2.13	0.47
1:D:302:PRO:HA	1:D:305:TYR:CD2	2.49	0.47
1:E:297:ARG:O	1:E:370:VAL:HA	2.14	0.47
1:A:10:SER:OG	1:A:307:ARG:HD2	2.15	0.47
1:A:41:GLY:O	1:A:51:TYR:HB2	2.15	0.47
1:E:194:ARG:HB3	1:E:200:GLU:CG	2.45	0.47
1:E:188:LEU:HA	1:E:354:PHE:O	2.14	0.47
1:B:376:THR:O	1:B:379:MET:HE2	2.15	0.47
1:E:195:ARG:NH2	1:E:197:TRP:CD2	2.83	0.47
1:E:95:VAL:HG21	1:E:140:LEU:CD1	2.44	0.47
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.15	0.47
1:A:230:GLY:O	2:A:394:PB8:H32	2.15	0.47
1:B:237:PRO:HA	1:B:327:SER:O	2.15	0.47
1:B:297:ARG:NH2	1:B:371:GLU:OE1	2.39	0.47
1:B:54:ARG:HD2	1:B:60:TYR:OH	2.15	0.47
1:D:183:LEU:HB2	1:D:342:TYR:CE2	2.50	0.47
1:D:261:PHE:CD1	1:D:268:VAL:HG23	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:VAL:HG11	1:D:136:PHE:CZ	2.50	0.47
1:E:188:LEU:HD23	1:E:354:PHE:C	2.35	0.47
1:E:280:PHE:HB2	1:E:302:PRO:HG3	1.96	0.47
1:E:32:ASP:C	1:E:34:GLY:N	2.69	0.47
1:E:26:THR:HG22	1:E:50:ARG:HH12	1.79	0.47
1:E:20:VAL:HG23	1:E:84:LEU:O	2.15	0.47
1:B:322:PHE:CE2	1:B:324:ILE:HB	2.50	0.47
1:D:202:ILE:HA	1:D:221:ASN:OD1	2.15	0.47
1:D:61:ARG:N	1:D:82:THR:O	2.48	0.46
1:B:30:LEU:HG	1:B:31:VAL:N	2.28	0.46
1:D:137:PHE:CD2	1:D:347:ARG:NE	2.83	0.46
1:A:364:GLU:O	1:B:374:PHE:CE1	2.69	0.46
1:D:241:PHE:CE1	1:D:324:ILE:HG22	2.49	0.46
1:D:234:LEU:HD22	1:D:337:ILE:HD11	1.97	0.46
1:D:381:ASP:C	1:D:381:ASP:OD1	2.53	0.46
1:B:190:TYR:CD1	1:B:351:ARG:HG3	2.51	0.46
1:A:251:ALA:HB3	1:A:281:PRO:HG3	1.97	0.46
1:D:194:ARG:HD3	1:D:200:GLU:OE1	2.16	0.46
1:D:83:ASP:OD1	1:D:84:LEU:N	2.49	0.46
1:E:123:TYR:O	1:E:124:ALA:C	2.53	0.46
1:A:234:LEU:O	1:A:324:ILE:HA	2.15	0.46
1:B:180:ASP:HB3	1:B:183:LEU:HD12	1.97	0.46
1:D:197:TRP:HD1	1:D:197:TRP:H	1.63	0.46
1:D:314:THR:O	1:D:314:THR:HG22	2.16	0.46
1:D:54:ARG:O	1:D:56:LEU:N	2.49	0.46
1:E:297:ARG:HB2	1:E:374:PHE:HE2	1.81	0.46
1:E:14:TYR:CD2	1:E:154:LEU:HG	2.51	0.46
1:E:42:ALA:HB3	1:E:102:ILE:O	2.15	0.46
1:A:149:LEU:O	1:A:177:GLY:N	2.48	0.46
1:A:98:ASN:ND2	3:A:399:HOH:O	2.19	0.46
1:D:327:SER:OG	1:D:330:GLY:O	2.24	0.46
1:D:199:TYR:HB3	1:D:352:ILE:HD11	1.98	0.46
1:B:302:PRO:C	1:B:304:GLN:H	2.17	0.46
1:D:61:ARG:O	1:D:81:GLY:HA2	2.16	0.46
1:E:126:ILE:HG23	1:E:197:TRP:HB2	1.98	0.46
1:A:311:ASP:OD1	1:A:312:VAL:N	2.49	0.45
1:A:341:PHE:HB3	1:A:355:ALA:O	2.16	0.45
1:B:148:ASN:HB3	1:B:348:ALA:HB2	1.97	0.45
1:B:204:VAL:HG11	1:B:379:MET:HG2	1.97	0.45
1:D:300:ILE:HG13	1:D:300:ILE:O	2.15	0.45
1:D:301:LEU:HA	1:D:302:PRO:HD2	1.68	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LYS:HE2	1:E:246:LYS:HA	1.98	0.45
1:E:99:ILE:HG22	1:E:100:ALA:C	2.37	0.45
1:A:10:SER:OG	1:A:11:GLY:N	2.50	0.45
1:E:114:ASN:ND2	1:E:167:LEU:HD21	2.31	0.45
1:A:130:ASP:CG	1:A:132:SER:H	2.18	0.45
1:A:288:MET:HG3	1:A:289:GLY:N	2.31	0.45
1:B:236:LEU:HD22	1:B:240:VAL:CG1	2.47	0.45
1:B:2:MET:CG	1:B:90:GLY:HA2	2.46	0.45
1:B:91:PRO:O	1:B:93:VAL:N	2.49	0.45
1:D:174:MET:O	1:D:174:MET:HG2	2.16	0.45
1:A:14:TYR:OH	1:A:339:GLU:OE2	2.33	0.45
1:B:68:TYR:OH	1:B:70:PRO:HG3	2.17	0.45
1:A:357:SER:OG	1:A:359:CYS:CB	2.65	0.45
1:E:231:THR:HG21	1:E:332:VAL:HG11	1.98	0.45
1:A:343:VAL:HG12	1:A:345:PHE:CE2	2.52	0.45
1:A:375:VAL:HG12	1:A:375:VAL:O	2.16	0.45
1:D:235:ARG:HB2	1:D:332:VAL:HB	1.98	0.45
1:E:297:ARG:NH2	1:E:371:GLU:OE1	2.49	0.45
1:A:344:VAL:HB	1:A:353:GLY:HA3	1.99	0.45
1:D:213:LEU:HD11	1:D:244:ALA:HA	1.99	0.45
1:E:194:ARG:HB3	1:E:200:GLU:HG2	1.99	0.45
1:A:4:ASP:CG	1:A:170:VAL:HG21	2.37	0.45
1:E:280:PHE:CB	1:E:302:PRO:HB3	2.46	0.45
1:E:21:GLY:HA2	1:E:57:SER:OG	2.16	0.45
1:E:61:ARG:HD2	1:E:96:ARG:CZ	2.46	0.45
1:B:205:ARG:NH2	1:B:212:ASP:HB2	2.31	0.45
1:D:45:HIS:CE1	1:D:46:PRO:HD2	2.52	0.45
1:A:222:TYR:O	1:A:330:GLY:CA	2.61	0.44
2:A:394:PB8:C28	2:A:394:PB8:H9	2.47	0.44
1:B:222:TYR:O	1:B:223:ASP:CB	2.64	0.44
1:D:6:LEU:HB2	1:D:172:GLY:C	2.38	0.44
1:A:357:SER:O	1:A:359:CYS:N	2.48	0.44
2:A:394:PB8:H37	2:A:394:PB8:H24A	1.64	0.44
1:D:3:VAL:O	1:D:4:ASP:HB2	2.17	0.44
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.72	0.44
1:D:191:THR:HA	1:D:192:PRO:HD3	1.83	0.44
1:D:45:HIS:CD2	1:D:46:PRO:HD2	2.52	0.44
1:E:203:ILE:HD13	1:E:285:LEU:HD13	1.99	0.44
1:A:242:GLU:O	1:A:245:VAL:HG12	2.17	0.44
1:B:180:ASP:HB3	1:B:183:LEU:CD1	2.47	0.44
1:D:51:TYR:H	1:D:51:TYR:HD2	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ALA:HB1	1:E:336:VAL:HG11	2.00	0.44
1:E:218:LYS:HG3	1:E:382:CYS:O	2.18	0.44
1:E:61:ARG:HD2	1:E:96:ARG:NH1	2.32	0.44
1:E:301:LEU:CB	1:E:302:PRO:HD2	2.47	0.44
1:B:40:VAL:HG12	1:B:117:GLY:HA3	1.98	0.44
1:B:322:PHE:CE1	1:B:324:ILE:HD12	2.52	0.44
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.77	0.44
1:D:84:LEU:HD23	1:D:96:ARG:HB2	1.99	0.44
1:A:54:ARG:O	1:A:55:GLN:C	2.56	0.44
1:D:112:GLY:O	1:D:163:GLN:OE1	2.36	0.44
1:D:148:ASN:HB3	1:D:348:ALA:HB2	2.00	0.44
1:E:234:LEU:O	1:E:324:ILE:HA	2.18	0.44
1:E:261:PHE:CD2	1:E:261:PHE:C	2.91	0.44
1:B:119:LEU:HD11	1:B:136:PHE:HB3	2.00	0.44
1:B:153:GLN:NE2	1:B:155:CYS:SG	2.90	0.44
1:B:23:PRO:HB2	1:B:24:PRO:HD2	2.00	0.44
1:D:2:MET:CE	1:D:91:PRO:CD	2.92	0.44
1:A:121:LEU:HD11	1:A:174:MET:CE	2.48	0.44
1:D:125:GLU:HG2	1:D:197:TRP:CB	2.47	0.44
1:D:45:HIS:ND1	1:D:46:PRO:CD	2.79	0.44
1:B:124:ALA:O	1:B:126:ILE:N	2.51	0.43
1:B:69:VAL:HG22	1:B:128:ARG:HG3	2.00	0.43
1:E:179:ILE:HD13	1:E:344:VAL:HG21	1.98	0.43
1:E:26:THR:CG2	1:E:50:ARG:HH12	2.30	0.43
1:D:188:LEU:HD12	1:D:188:LEU:HA	1.79	0.43
1:D:197:TRP:CD2	1:D:198:TYR:HD2	2.37	0.43
1:D:261:PHE:HZ	1:D:306:LEU:HD21	1.82	0.43
1:D:38:PHE:CD1	1:D:119:LEU:HD12	2.53	0.43
1:D:80:LEU:HA	1:D:80:LEU:HD23	1.43	0.43
1:B:133:LEU:O	1:B:135:PRO:HD3	2.19	0.43
1:B:149:LEU:HD21	1:B:179:ILE:HG13	2.00	0.43
1:D:197:TRP:N	1:D:197:TRP:HD1	2.14	0.43
1:D:242:GLU:HG2	1:D:242:GLU:H	1.41	0.43
1:D:266:GLN:HG3	1:D:267:LEU:O	2.19	0.43
1:E:244:ALA:O	1:E:248:ILE:HG13	2.18	0.43
1:E:45:HIS:HE1	1:E:47:PHE:CD2	2.36	0.43
1:E:83:ASP:OD1	1:E:84:LEU:N	2.48	0.43
1:D:18:MET:CE	1:D:119:LEU:HD13	2.48	0.43
1:E:85:VAL:N	1:E:95:VAL:O	2.49	0.43
1:A:209:ASN:OD1	1:A:281:PRO:HA	2.18	0.43
1:A:3:VAL:O	1:A:4:ASP:HB2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG13	1:B:366:ARG:HH11	1.84	0.43
1:E:137:PHE:HE1	1:E:176:ILE:HG23	1.83	0.43
1:A:121:LEU:HD11	1:A:174:MET:HE1	2.00	0.43
1:B:126:ILE:HD13	1:B:198:TYR:CD1	2.54	0.43
1:D:197:TRP:CG	1:D:198:TYR:N	2.85	0.43
1:A:162:ASN:O	1:A:165:GLU:N	2.51	0.43
1:A:73:GLN:HE21	2:A:394:PB8:H5	1.82	0.43
1:A:45:HIS:CB	1:A:48:LEU:HD12	2.49	0.43
1:A:20:VAL:CG2	1:A:52:TYR:CE1	3.02	0.43
1:D:244:ALA:O	1:D:248:ILE:HG13	2.19	0.43
1:E:27:LEU:HD22	1:E:116:GLU:OE1	2.18	0.43
1:D:91:PRO:O	1:D:93:VAL:N	2.48	0.43
1:A:277:TRP:HE3	1:A:302:PRO:HB2	1.83	0.43
1:B:162:ASN:O	1:B:165:GLU:N	2.51	0.43
1:B:259:ASP:HA	1:B:262:TRP:HD1	1.84	0.43
1:D:267:LEU:CD2	1:D:321:LYS:HG3	2.48	0.43
1:D:85:VAL:HB	1:D:95:VAL:HG13	2.00	0.43
1:E:162:ASN:OD1	1:E:164:SER:HB3	2.19	0.43
1:E:301:LEU:HB3	1:E:302:PRO:HD2	2.01	0.43
1:B:190:TYR:HA	1:B:352:ILE:O	2.19	0.42
1:B:22:SER:HA	1:B:23:PRO:HA	1.86	0.42
1:D:267:LEU:HD22	1:D:321:LYS:HG3	1.99	0.42
1:A:165:GLU:O	1:A:169:SER:N	2.50	0.42
1:B:85:VAL:HG12	1:B:86:SER:N	2.33	0.42
1:D:29:ILE:HD13	1:D:29:ILE:N	2.34	0.42
1:B:235:ARG:NH2	2:B:394:PB8:H8	2.34	0.42
1:A:-1:PHE:CE2	1:A:178:GLY:HA3	2.54	0.42
1:B:236:LEU:HD22	1:B:240:VAL:HG11	2.01	0.42
1:B:202:ILE:HG21	1:B:382:CYS:HB2	2.01	0.42
1:E:261:PHE:CD1	1:E:268:VAL:HG23	2.55	0.42
1:E:71:TYR:CB	2:E:394:PB8:H11	2.50	0.42
1:E:83:ASP:O	1:E:96:ARG:HA	2.19	0.42
1:B:223:ASP:HA	1:B:384:TYR:CD2	2.54	0.42
1:E:179:ILE:CD1	1:E:344:VAL:HG21	2.49	0.42
1:E:32:ASP:HA	1:E:229:SER:OG	2.19	0.42
1:A:224:LYS:O	1:A:330:GLY:HA3	2.19	0.42
1:B:2:MET:SD	1:B:91:PRO:HD3	2.60	0.42
1:A:149:LEU:O	1:A:149:LEU:HD12	2.19	0.42
1:A:349:ARG:HD2	3:A:417:HOH:O	2.19	0.42
1:E:235:ARG:HA	1:E:325:SER:O	2.20	0.42
1:E:340:GLY:HA2	1:E:360:HIS:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:HB	1:A:145:HIS:H	1.48	0.42
1:B:267:LEU:CD1	1:B:269:CYS:SG	3.06	0.42
1:D:175:ILE:HD13	1:D:175:ILE:N	2.35	0.42
1:E:140:LEU:HD12	1:E:140:LEU:C	2.40	0.42
2:D:394:PB8:H37	2:D:394:PB8:O43	2.20	0.42
2:A:394:PB8:H28A	2:A:394:PB8:H9	2.00	0.42
1:D:189:TRP:CD1	1:D:370:VAL:HG12	2.55	0.42
1:E:16:VAL:HG21	1:E:174:MET:HE1	2.01	0.42
1:A:251:ALA:C	1:A:253:SER:H	2.21	0.41
1:A:32:ASP:OD1	1:A:230:GLY:HA3	2.20	0.41
1:D:188:LEU:CD1	1:D:355:ALA:CB	2.95	0.41
1:D:359:CYS:O	1:D:359:CYS:SG	2.77	0.41
1:E:208:ILE:HG21	1:E:247:SER:HB3	2.01	0.41
1:A:267:LEU:HD12	1:A:267:LEU:C	2.41	0.41
1:A:283:ILE:HB	1:A:300:ILE:HD11	2.02	0.41
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.35	0.41
1:B:298:ILE:HB	1:B:341:PHE:CZ	2.55	0.41
1:B:45:HIS:CD2	1:B:46:PRO:HD2	2.55	0.41
1:D:37:ASN:HD21	1:D:127:ALA:HA	1.84	0.41
1:D:157:ALA:O	1:D:159:PHE:CE2	2.73	0.41
1:E:110:ILE:O	1:E:113:SER:HB3	2.20	0.41
1:B:239:LYS:NZ	1:B:239:LYS:HB3	2.35	0.41
1:B:63:LEU:HD12	1:B:80:LEU:HB3	2.00	0.41
1:D:137:PHE:HD2	1:D:347:ARG:NE	2.19	0.41
1:E:27:LEU:HB3	1:E:116:GLU:OE1	2.20	0.41
1:E:267:LEU:HD12	1:E:267:LEU:O	2.20	0.41
1:E:306:LEU:HA	1:E:306:LEU:HD23	1.83	0.41
1:E:293:ASN:C	1:E:379:MET:HE3	2.41	0.41
1:A:261:PHE:CZ	1:A:322:PHE:HB2	2.55	0.41
1:D:36:SER:OG	1:D:126:ILE:HG13	2.20	0.41
1:D:26:THR:HG22	1:D:50:ARG:NH1	2.35	0.41
1:E:14:TYR:OH	1:E:155:CYS:O	2.32	0.41
1:A:379:MET:O	1:A:381:ASP:N	2.54	0.41
1:B:203:ILE:HD11	1:B:331:THR:HG21	2.02	0.41
1:B:286:TYR:CZ	1:B:297:ARG:HD3	2.56	0.41
1:D:113:SER:O	1:D:114:ASN:HB3	2.20	0.41
1:D:240:VAL:O	1:D:241:PHE:C	2.58	0.41
1:D:222:TYR:O	1:D:330:GLY:HA2	2.21	0.41
1:A:199:TYR:O	1:A:226:ILE:HA	2.21	0.41
1:E:110:ILE:CD1	2:E:394:PB8:C30	2.99	0.41
1:A:20:VAL:HG23	1:A:52:TYR:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:O	1:A:292:THR:C	2.59	0.41
1:B:205:ARG:HB3	1:B:286:TYR:HB2	2.02	0.41
1:A:232:THR:HG22	1:A:233:ASN:OD1	2.20	0.41
1:D:134:GLU:HA	1:D:135:PRO:HD3	1.82	0.41
1:D:183:LEU:HB2	1:D:342:TYR:CD2	2.56	0.41
1:E:234:LEU:HB2	1:E:337:ILE:CD1	2.46	0.41
1:D:233:ASN:HD22	1:D:325:SER:HG	1.64	0.41
1:D:85:VAL:N	1:D:95:VAL:O	2.45	0.41
1:E:199:TYR:HB3	1:E:352:ILE:HD11	2.02	0.41
1:E:299:THR:O	1:E:368:ALA:HB1	2.21	0.41
1:A:249:LYS:HE2	1:A:262:TRP:CG	2.56	0.41
1:A:206:VAL:HG22	1:A:285:LEU:CD2	2.51	0.41
1:B:125:GLU:HA	1:B:131:ASP:HB3	2.02	0.41
1:B:130:ASP:C	1:B:132:SER:H	2.25	0.41
1:E:334:GLY:O	1:E:337:ILE:N	2.54	0.41
1:A:207:GLU:HA	1:A:211:GLN:O	2.21	0.41
1:B:14:TYR:CD2	1:B:154:LEU:HG	2.55	0.41
1:E:218:LYS:CE	1:E:381:ASP:O	2.69	0.41
1:A:140:LEU:HD21	1:A:176:ILE:HG21	2.03	0.40
1:B:284:SER:HA	1:B:298:ILE:O	2.21	0.40
1:D:221:ASN:N	1:D:221:ASN:HD22	2.19	0.40
1:E:162:ASN:O	1:E:163:GLN:C	2.60	0.40
1:E:270:TRP:CE3	1:E:275:THR:HG23	2.56	0.40
1:A:137:PHE:CE1	1:A:150:PHE:HB3	2.55	0.40
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.84	0.40
1:B:208:ILE:O	1:B:209:ASN:C	2.59	0.40
1:E:234:LEU:HD23	1:E:324:ILE:HG21	2.03	0.40
1:E:222:TYR:O	1:E:330:GLY:HA2	2.21	0.40
1:A:162:ASN:O	1:A:166:VAL:HG12	2.22	0.40
1:A:205:ARG:HG2	1:A:286:TYR:CD2	2.56	0.40
1:B:302:PRO:C	1:B:304:GLN:N	2.74	0.40
1:B:342:TYR:N	1:B:355:ALA:O	2.53	0.40
1:B:357:SER:C	1:B:359:CYS:N	2.75	0.40
1:D:45:HIS:CG	1:D:46:PRO:CD	2.99	0.40
1:A:17:GLU:HG2	1:A:88:PRO:HG2	2.03	0.40
1:D:9:LYS:HD3	1:D:166:VAL:HG22	2.03	0.40
1:D:194:ARG:HH22	1:D:384:TYR:N	2.19	0.40
1:D:22:SER:CB	1:D:59:THR:CG2	2.99	0.40
1:A:153:GLN:HG2	1:A:155:CYS:SG	2.62	0.40
2:A:394:PB8:H28B	2:A:394:PB8:H24	2.04	0.40
1:D:184:TYR:CD2	1:D:342:TYR:HD2	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:VAL:HG13	1:E:366:ARG:NH1	2.36	0.40
1:E:366:ARG:HD3	3:E:417:HOH:O	2.21	0.40
1:E:235:ARG:CZ	2:E:394:PB8:H8	2.52	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	384/455 (84%)	338 (88%)	39 (10%)	7 (2%)	8	27
1	B	384/455 (84%)	338 (88%)	42 (11%)	4 (1%)	15	42
1	D	384/455 (84%)	336 (88%)	37 (10%)	11 (3%)	4	16
1	E	384/455 (84%)	337 (88%)	38 (10%)	9 (2%)	6	21
All	All	1536/1820 (84%)	1349 (88%)	156 (10%)	31 (2%)	7	25

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	107	LYS
1	D	55	GLN
1	D	92	ASN
1	D	380	GLU
1	E	217	CYS
1	E	223	ASP
1	E	254	THR
1	E	271	GLN
1	E	278	ASN
1	A	60	TYR
1	B	217	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	223	ASP
1	B	358	ALA
1	D	122	ALA
1	D	166	VAL
1	D	378	ASP
1	E	358	ALA
1	A	217	CYS
1	D	125	GLU
1	A	277	TRP
1	A	358	ALA
1	D	58	SER
1	D	254	THR
1	E	163	GLN
1	A	380	GLU
1	B	314	THR
1	D	271	GLN
1	E	0	VAL
1	E	312	VAL
1	D	0	VAL

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	329/381 (86%)	294 (89%)	35 (11%)	6 19
1	B	329/381 (86%)	290 (88%)	39 (12%)	5 14
1	D	329/381 (86%)	282 (86%)	47 (14%)	3 9
1	E	329/381 (86%)	289 (88%)	40 (12%)	5 13
All	All	1316/1524 (86%)	1155 (88%)	161 (12%)	5 13

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	2	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	SER
1	A	20	VAL
1	A	25	GLN
1	A	27	LEU
1	A	73	GLN
1	A	75	LYS
1	A	130	ASP
1	A	131	ASP
1	A	161	LEU
1	A	162	ASN
1	A	163	GLN
1	A	166	VAL
1	A	167	LEU
1	A	170	VAL
1	A	174	MET
1	A	194	ARG
1	A	197	TRP
1	A	213	LEU
1	A	217	CYS
1	A	232	THR
1	A	239	LYS
1	A	265	GLU
1	A	267	LEU
1	A	278	ASN
1	A	288	MET
1	A	300	ILE
1	A	308	PRO
1	A	327	SER
1	A	328	SER
1	A	349	ARG
1	A	367	THR
1	A	377	LEU
1	A	381	ASP
1	B	10	SER
1	B	18	MET
1	B	59	THR
1	B	68	TYR
1	B	73	GLN
1	B	75	LYS
1	B	77	GLU
1	B	82	THR
1	B	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	106	ASP
1	B	132	SER
1	B	137	PHE
1	B	139	SER
1	B	152	LEU
1	B	153	GLN
1	B	154	LEU
1	B	167	LEU
1	B	169	SER
1	B	176	ILE
1	B	187	SER
1	B	197	TRP
1	B	214	LYS
1	B	217	CYS
1	B	218	LYS
1	B	239	LYS
1	B	256	LYS
1	B	266	GLN
1	B	292	THR
1	B	293	ASN
1	B	301	LEU
1	B	314	THR
1	B	315	SER
1	B	316	GLN
1	B	325	SER
1	B	327	SER
1	B	329	THR
1	B	337	ILE
1	B	359	CYS
1	B	367	THR
1	D	9	LYS
1	D	26	THR
1	D	51	TYR
1	D	59	THR
1	D	65	LYS
1	D	68	TYR
1	D	75	LYS
1	D	94	THR
1	D	125	GLU
1	D	128	ARG
1	D	130	ASP
1	D	144	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	154	LEU
1	D	159	PHE
1	D	169	SER
1	D	176	ILE
1	D	185	THR
1	D	187	SER
1	D	188	LEU
1	D	197	TRP
1	D	204	VAL
1	D	213	LEU
1	D	214	LYS
1	D	221	ASN
1	D	238	LYS
1	D	246	LYS
1	D	247	SER
1	D	249	LYS
1	D	252	SER
1	D	259	ASP
1	D	263	LEU
1	D	266	GLN
1	D	284	SER
1	D	292	THR
1	D	296	PHE
1	D	299	THR
1	D	309	VAL
1	D	311	ASP
1	D	315	SER
1	D	328	SER
1	D	329	THR
1	D	341	PHE
1	D	362	HIS
1	D	367	THR
1	D	373	PRO
1	D	375	VAL
1	D	382	CYS
1	E	1	GLU
1	E	17	GLU
1	E	48	LEU
1	E	55	GLN
1	E	56	LEU
1	E	63	LEU
1	E	65	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	75	LYS
1	E	85	VAL
1	E	87	ILE
1	E	99	ILE
1	E	104	GLU
1	E	105	SER
1	E	116	GLU
1	E	154	LEU
1	E	176	ILE
1	E	183	LEU
1	E	193	ILE
1	E	195	ARG
1	E	197	TRP
1	E	200	GLU
1	E	217	CYS
1	E	239	LYS
1	E	247	SER
1	E	253	SER
1	E	298	ILE
1	E	300	ILE
1	E	301	LEU
1	E	312	VAL
1	E	314	THR
1	E	317	ASP
1	E	324	ILE
1	E	362	HIS
1	E	363	ASP
1	E	364	GLU
1	E	367	THR
1	E	376	THR
1	E	379	MET
1	E	380	GLU
1	E	381	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	162	ASN
1	A	211	GLN
1	A	271	GLN
1	B	143	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	GLN
1	B	211	GLN
1	B	360	HIS
1	D	37	ASN
1	D	111	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	PB8	E	394	-	52,52,52	1.92	15 (28%)	60,74,74	2.93	28 (46%)
2	PB8	D	394	-	52,52,52	2.15	12 (23%)	60,74,74	2.93	28 (46%)
2	PB8	A	394	-	52,52,52	2.19	12 (23%)	60,74,74	2.48	22 (36%)
2	PB8	B	394	-	52,52,52	2.00	13 (25%)	60,74,74	2.92	26 (43%)

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	PB8	E	394	-	-	14/39/64/64	0/5/5/5
2	PB8	D	394	-	-	6/39/64/64	0/5/5/5
2	PB8	A	394	-	-	6/39/64/64	0/5/5/5
2	PB8	B	394	-	-	18/39/64/64	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	394	PB8	C7-C14	7.55	1.52	1.39
2	E	394	PB8	C27-C19	-5.84	1.47	1.52
2	D	394	PB8	C14-C13	-5.58	1.29	1.40
2	B	394	PB8	C6-C13	5.54	1.49	1.39
2	D	394	PB8	C27-C19	-5.54	1.47	1.52
2	A	394	PB8	C14-C13	-5.39	1.29	1.40
2	B	394	PB8	C14-C13	-5.38	1.29	1.40
2	D	394	PB8	C7-C14	5.31	1.48	1.39
2	B	394	PB8	C7-C14	5.18	1.48	1.39
2	E	394	PB8	C7-C14	5.01	1.48	1.39
2	A	394	PB8	C6-C13	4.99	1.48	1.39
2	A	394	PB8	C23-N39	4.97	1.53	1.46
2	D	394	PB8	C3-C2	4.80	1.50	1.38
2	A	394	PB8	C26-N39	4.78	1.54	1.47
2	D	394	PB8	C6-C13	4.47	1.47	1.39
2	B	394	PB8	C3-C2	4.22	1.49	1.38
2	B	394	PB8	C2-C6	-4.19	1.30	1.38
2	D	394	PB8	C3-C7	-3.82	1.30	1.38
2	A	394	PB8	C3-C2	3.81	1.48	1.38
2	E	394	PB8	C3-C2	3.62	1.47	1.38
2	D	394	PB8	C12-C17	3.61	1.43	1.37
2	D	394	PB8	C26-N39	3.59	1.52	1.47
2	D	394	PB8	C35-N40	-3.52	1.41	1.46
2	E	394	PB8	C2-C6	-3.40	1.31	1.38
2	B	394	PB8	C36-C38	3.37	1.59	1.53
2	E	394	PB8	C26-N39	3.36	1.52	1.47
2	D	394	PB8	C2-C6	-3.35	1.31	1.38
2	E	394	PB8	C6-C13	3.30	1.45	1.39
2	B	394	PB8	C23-N39	3.25	1.51	1.46
2	E	394	PB8	C3-C7	-3.25	1.32	1.38
2	B	394	PB8	C35-N40	3.19	1.50	1.46
2	E	394	PB8	C34-C35	-3.19	1.48	1.53
2	E	394	PB8	C14-C13	-3.02	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	394	PB8	C5-C1	2.83	1.45	1.38
2	A	394	PB8	C35-N40	-2.82	1.42	1.46
2	B	394	PB8	C3-C7	-2.57	1.33	1.38
2	B	394	PB8	C20-N41	2.42	1.38	1.34
2	B	394	PB8	C32-C38	-2.41	1.48	1.53
2	B	394	PB8	C28-C20	2.38	1.55	1.50
2	E	394	PB8	C35-N40	-2.36	1.43	1.46
2	A	394	PB8	C36-C26	2.34	1.57	1.53
2	A	394	PB8	C27-C19	-2.28	1.50	1.52
2	E	394	PB8	C20-N41	2.27	1.38	1.34
2	D	394	PB8	O45-C21	-2.26	1.18	1.23
2	E	394	PB8	C23-N39	2.25	1.49	1.46
2	E	394	PB8	F48-C18	-2.22	1.31	1.36
2	A	394	PB8	C3-C7	-2.18	1.34	1.38
2	E	394	PB8	C8-C15	2.16	1.43	1.38
2	A	394	PB8	C2-C6	-2.12	1.34	1.38
2	B	394	PB8	C11-C16	-2.05	1.35	1.39
2	E	394	PB8	C35-C21	-2.04	1.48	1.52
2	D	394	PB8	C9-C15	2.04	1.43	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	394	PB8	O43-C19-C27	-10.17	118.06	126.67
2	B	394	PB8	C25-N40-C19	-9.77	107.14	113.43
2	B	394	PB8	C28-C20-N41	9.24	127.95	115.98
2	E	394	PB8	O43-C19-C27	-8.71	119.30	126.67
2	E	394	PB8	C16-C10-C17	8.27	126.33	118.81
2	A	394	PB8	C28-C20-N41	7.96	126.30	115.98
2	D	394	PB8	C27-C33-C37	-7.06	105.34	118.46
2	D	394	PB8	C28-C20-N41	6.76	124.75	115.98
2	B	394	PB8	C12-C17-C10	-6.47	115.35	123.52
2	E	394	PB8	C12-C17-C10	-6.42	115.41	123.52
2	E	394	PB8	F47-C17-C12	6.14	127.03	118.25
2	D	394	PB8	C27-N41-C20	6.09	131.79	123.03
2	A	394	PB8	C27-C33-C37	-5.60	108.06	118.46
2	A	394	PB8	C24-C25-N40	5.54	109.42	103.21
2	D	394	PB8	C32-C38-N42	-5.34	102.28	110.07
2	A	394	PB8	C16-C11-C18	5.08	123.43	118.81
2	E	394	PB8	C34-C31-C15	-5.07	95.57	113.18
2	E	394	PB8	C25-N40-C19	-5.05	110.18	113.43
2	A	394	PB8	C27-N41-C20	5.00	130.23	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	394	PB8	C16-C10-C17	4.86	123.23	118.81
2	B	394	PB8	C24-C25-N40	4.77	108.55	103.21
2	B	394	PB8	O44-C20-C28	-4.60	113.51	122.06
2	D	394	PB8	C14-C23-N39	-4.60	102.67	113.42
2	E	394	PB8	C27-N41-C20	4.60	129.64	123.03
2	A	394	PB8	C2-C3-C7	-4.58	113.21	120.19
2	E	394	PB8	C32-C38-C36	-4.40	102.04	111.11
2	A	394	PB8	O44-C20-N41	-4.35	116.36	122.28
2	B	394	PB8	C33-C27-N41	4.34	118.18	108.97
2	E	394	PB8	C28-C20-N41	4.28	121.53	115.98
2	B	394	PB8	F47-C17-C12	4.27	124.36	118.25
2	D	394	PB8	O43-C19-N40	4.19	131.78	126.19
2	B	394	PB8	C27-N41-C20	3.93	128.68	123.03
2	E	394	PB8	C13-C22-C26	-3.82	106.78	113.69
2	B	394	PB8	C35-N40-C19	3.77	126.71	122.03
2	E	394	PB8	C14-C23-N39	-3.76	104.64	113.42
2	D	394	PB8	C12-C17-C10	-3.73	118.81	123.52
2	B	394	PB8	C18-C12-C17	3.67	121.84	116.13
2	D	394	PB8	C12-C18-C11	-3.65	118.91	123.52
2	E	394	PB8	O44-C20-C28	-3.60	115.36	122.06
2	D	394	PB8	C2-C3-C7	-3.58	114.74	120.19
2	D	394	PB8	C34-C35-N40	-3.52	108.63	112.65
2	D	394	PB8	O46-C36-C26	-3.49	100.63	108.98
2	D	394	PB8	C24-C27-N41	3.49	116.57	110.21
2	D	394	PB8	C32-C16-C10	-3.47	114.48	120.44
2	B	394	PB8	O46-C36-C38	3.43	117.17	108.98
2	B	394	PB8	C38-N42-C21	-3.41	117.05	123.07
2	A	394	PB8	O46-C36-C26	3.37	117.03	108.98
2	B	394	PB8	C16-C11-C18	-3.31	115.80	118.81
2	D	394	PB8	O44-C20-C28	-3.28	115.96	122.06
2	A	394	PB8	C25-N40-C19	-3.26	111.33	113.43
2	B	394	PB8	C32-C16-C10	-3.23	114.89	120.44
2	D	394	PB8	C7-C14-C13	3.20	122.91	118.98
2	B	394	PB8	C32-C38-N42	-3.17	105.45	110.07
2	D	394	PB8	C18-C12-C17	3.15	121.04	116.13
2	A	394	PB8	O43-C19-C27	-3.14	124.01	126.67
2	D	394	PB8	F47-C17-C12	3.12	122.72	118.25
2	E	394	PB8	F48-C18-C11	-3.02	113.94	118.25
2	E	394	PB8	C38-N42-C21	2.98	128.34	123.07
2	A	394	PB8	C3-C7-C14	2.96	125.32	120.89
2	E	394	PB8	C24-C27-N41	2.95	115.58	110.21
2	A	394	PB8	C32-C38-N42	-2.91	105.83	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	394	PB8	C1-C4-C8	-2.90	115.78	120.19
2	A	394	PB8	C9-C15-C8	2.83	122.62	118.17
2	D	394	PB8	C34-C31-C15	-2.80	103.43	113.18
2	B	394	PB8	O44-C20-N41	-2.75	118.54	122.28
2	E	394	PB8	C16-C11-C18	-2.74	116.32	118.81
2	B	394	PB8	C14-C23-N39	-2.71	107.09	113.42
2	E	394	PB8	C25-N40-C35	2.69	128.12	123.57
2	E	394	PB8	C34-C35-N40	-2.67	109.60	112.65
2	A	394	PB8	C30-C37-C29	-2.67	98.20	110.51
2	E	394	PB8	O45-C21-C35	2.63	127.17	120.63
2	A	394	PB8	C34-C35-N40	-2.59	109.69	112.65
2	D	394	PB8	C4-C8-C15	-2.59	116.65	120.63
2	B	394	PB8	O43-C19-N40	-2.57	122.77	126.19
2	E	394	PB8	C32-C16-C11	2.54	124.80	120.44
2	A	394	PB8	O44-C20-C28	-2.54	117.34	122.06
2	E	394	PB8	C27-C33-C37	-2.51	113.80	118.46
2	E	394	PB8	C23-C14-C7	-2.50	115.77	121.01
2	E	394	PB8	C16-C32-C38	-2.47	109.05	113.33
2	B	394	PB8	O45-C21-N42	-2.46	118.36	122.93
2	E	394	PB8	C22-C13-C6	-2.44	114.92	121.58
2	D	394	PB8	C13-C22-C26	-2.39	109.37	113.69
2	E	394	PB8	C1-C4-C8	-2.38	116.56	120.19
2	B	394	PB8	C21-C35-N40	-2.38	106.24	111.86
2	E	394	PB8	C12-C18-C11	2.37	126.50	123.52
2	E	394	PB8	C22-C13-C14	2.32	125.27	120.30
2	A	394	PB8	C22-C13-C14	2.27	125.16	120.30
2	B	394	PB8	O45-C21-C35	2.23	126.18	120.63
2	B	394	PB8	C5-C9-C15	-2.21	117.24	120.63
2	D	394	PB8	O44-C20-N41	-2.21	119.28	122.28
2	D	394	PB8	C32-C16-C11	2.20	124.20	120.44
2	A	394	PB8	C5-C9-C15	-2.19	117.27	120.63
2	D	394	PB8	F48-C18-C11	2.18	121.36	118.25
2	A	394	PB8	O45-C21-N42	-2.17	118.92	122.93
2	D	394	PB8	C9-C15-C8	2.16	121.56	118.17
2	B	394	PB8	C1-C5-C9	2.15	123.47	120.19
2	D	394	PB8	C22-C13-C14	2.14	124.88	120.30
2	D	394	PB8	C33-C27-N41	2.13	113.51	108.97
2	D	394	PB8	C6-C13-C14	-2.12	116.37	118.98
2	E	394	PB8	C30-C37-C29	-2.10	100.82	110.51
2	A	394	PB8	C13-C22-C26	2.10	117.48	113.69
2	B	394	PB8	C2-C6-C13	2.10	124.02	120.89
2	B	394	PB8	C34-C35-N40	2.07	115.01	112.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	394	PB8	C34-C31-C15	-2.02	106.16	113.18

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	394	PB8	C28-C20-N41-C27
2	E	394	PB8	O44-C20-N41-C27
2	E	394	PB8	C19-C27-C33-C37
2	E	394	PB8	C24-C27-C33-C37
2	E	394	PB8	C31-C34-C35-N40
2	E	394	PB8	C21-C35-N40-C19
2	E	394	PB8	C34-C35-N40-C19
2	D	394	PB8	C28-C20-N41-C27
2	D	394	PB8	O44-C20-N41-C27
2	A	394	PB8	C28-C20-N41-C27
2	A	394	PB8	O44-C20-N41-C27
2	A	394	PB8	N39-C26-C36-O46
2	B	394	PB8	C28-C20-N41-C27
2	B	394	PB8	O44-C20-N41-C27
2	B	394	PB8	C19-C27-C33-C37
2	B	394	PB8	C24-C27-C33-C37
2	B	394	PB8	C24-C27-N41-C20
2	B	394	PB8	C31-C34-C35-N40
2	B	394	PB8	C34-C35-N40-C25
2	B	394	PB8	O46-C36-C38-N42
2	E	394	PB8	C24-C27-N41-C20
2	B	394	PB8	C27-C33-C37-C30
2	E	394	PB8	C34-C35-N40-C25
2	A	394	PB8	N39-C26-C36-C38
2	D	394	PB8	C31-C34-C35-N40
2	E	394	PB8	C21-C35-N40-C25
2	B	394	PB8	C21-C35-N40-C25
2	B	394	PB8	C10-C16-C32-C38
2	A	394	PB8	C10-C16-C32-C38
2	A	394	PB8	C11-C16-C32-C38
2	B	394	PB8	C19-C27-N41-C20
2	D	394	PB8	C11-C16-C32-C38
2	D	394	PB8	C10-C16-C32-C38
2	B	394	PB8	C11-C16-C32-C38
2	E	394	PB8	N41-C27-C33-C37
2	B	394	PB8	N41-C27-C33-C37

Continued on next page...

Continued from previous page...

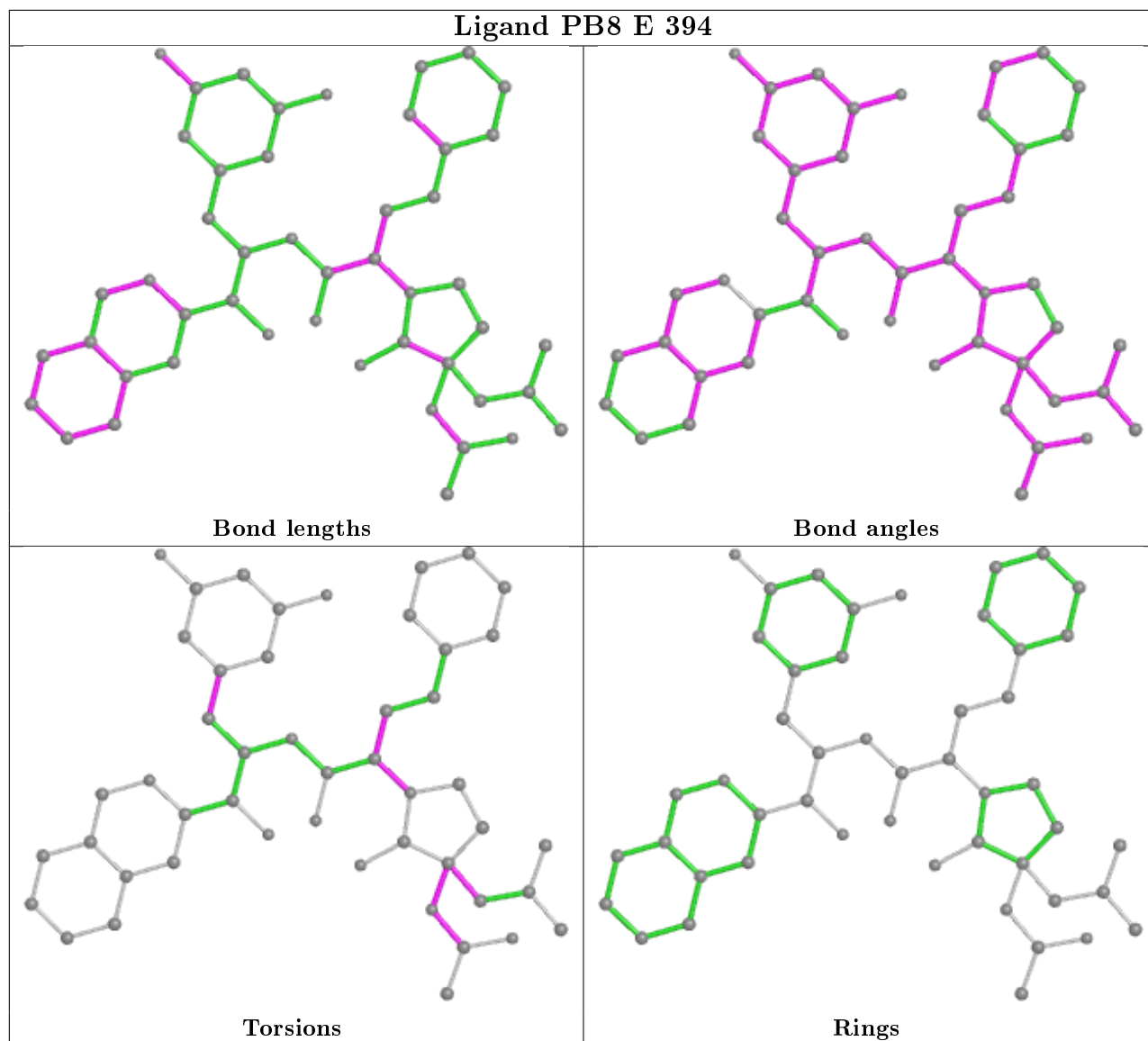
Mol	Chain	Res	Type	Atoms
2	E	394	PB8	C31-C34-C35-C21
2	E	394	PB8	C10-C16-C32-C38
2	E	394	PB8	C11-C16-C32-C38
2	B	394	PB8	C33-C27-N41-C20
2	D	394	PB8	C21-C35-N40-C25
2	B	394	PB8	C22-C26-C36-O46
2	B	394	PB8	N39-C26-C36-O46
2	B	394	PB8	C9-C15-C31-C34

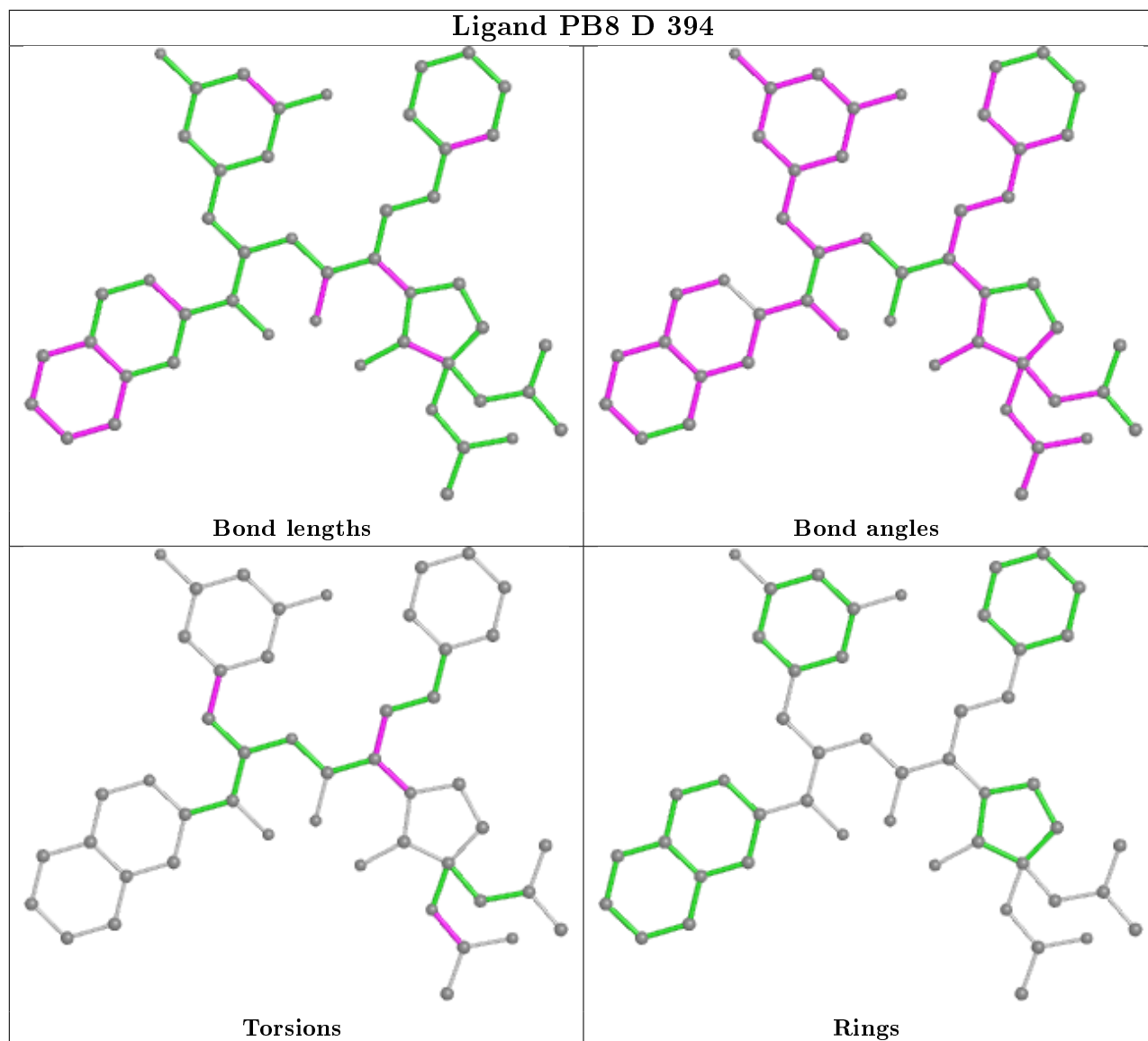
There are no ring outliers.

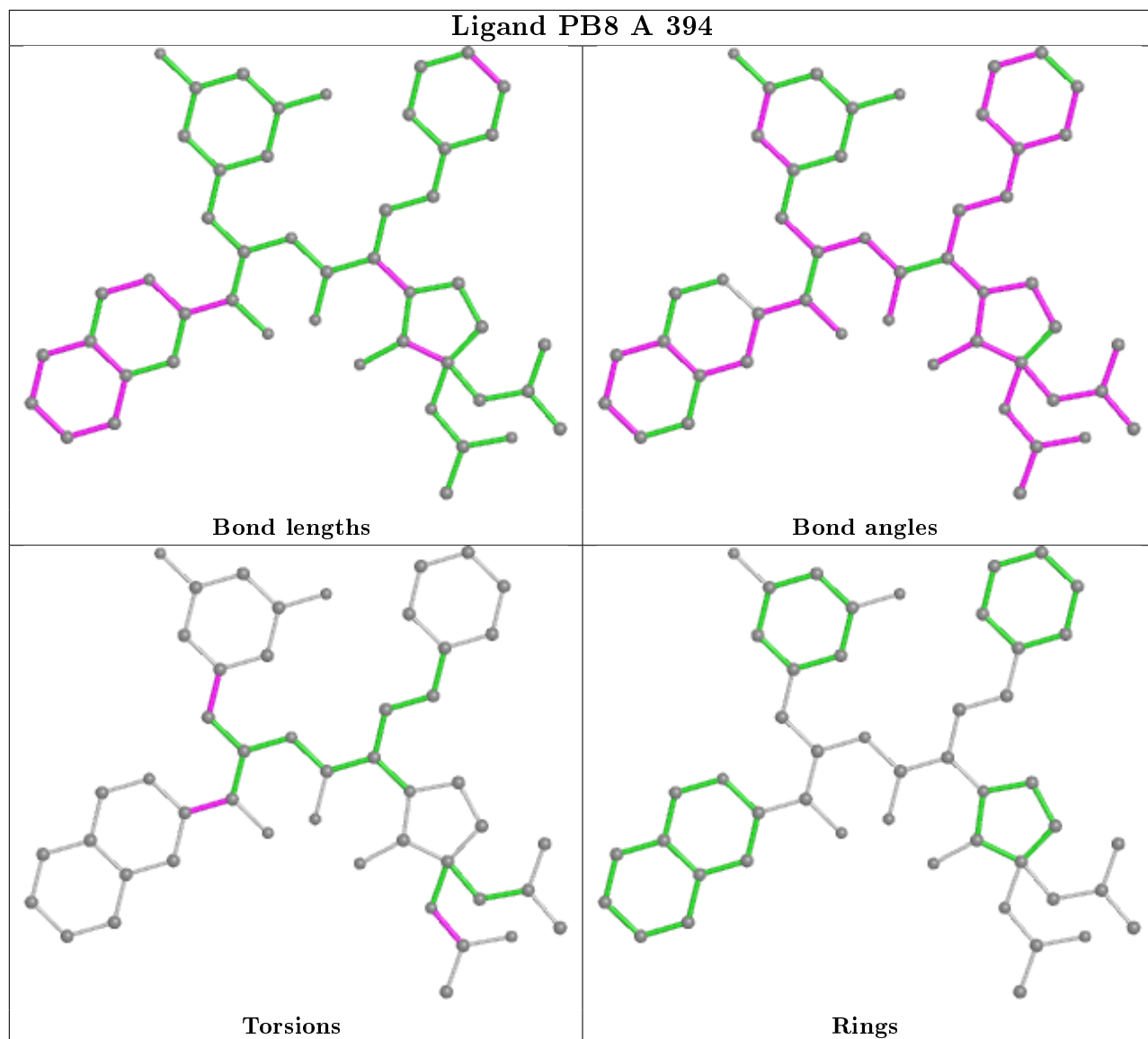
4 monomers are involved in 31 short contacts:

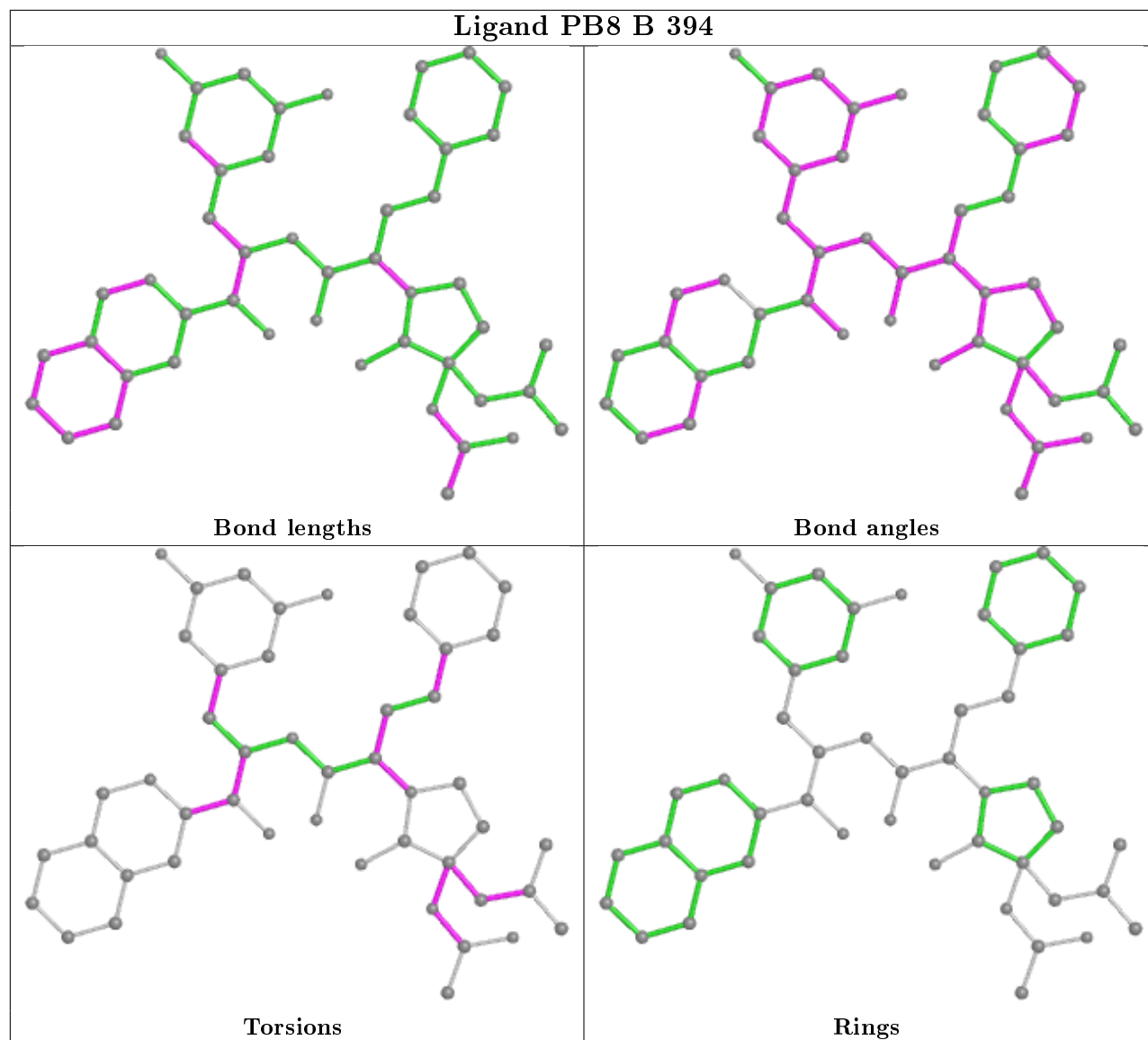
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	394	PB8	10	0
2	D	394	PB8	5	0
2	A	394	PB8	9	0
2	B	394	PB8	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/455 (84%)	0.17	12 (3%) 49 45	4, 18, 36, 59	0
1	B	386/455 (84%)	0.12	11 (2%) 53 50	3, 16, 35, 47	0
1	D	386/455 (84%)	0.45	24 (6%) 20 16	10, 24, 39, 59	0
1	E	386/455 (84%)	0.42	24 (6%) 20 16	10, 23, 41, 57	0
All	All	1544/1820 (84%)	0.29	71 (4%) 32 28	3, 20, 38, 59	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	5.7
1	E	378	ASP	4.8
1	E	311	ASP	4.8
1	B	313	ALA	4.6
1	A	376	THR	4.0
1	D	185	THR	3.9
1	E	376	THR	3.9
1	E	103	THR	3.8
1	E	380	GLU	3.8
1	B	376	THR	3.7
1	D	378	ASP	3.7
1	D	258	PRO	3.6
1	D	377	LEU	3.6
1	D	384	TYR	3.5
1	A	377	LEU	3.5
1	E	377	LEU	3.3
1	D	186	GLY	3.3
1	D	68	TYR	3.2
1	A	313	ALA	3.2
1	E	49	HIS	3.1
1	E	384	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	258	PRO	3.0
1	D	66	GLY	2.9
1	E	315	SER	2.9
1	E	312	VAL	2.9
1	E	0	VAL	2.9
1	D	293	ASN	2.9
1	D	103	THR	2.8
1	E	145	HIS	2.8
1	E	313	ALA	2.8
1	E	181	HIS	2.7
1	A	378	ASP	2.7
1	A	312	VAL	2.7
1	B	380	GLU	2.6
1	A	380	GLU	2.6
1	B	259	ASP	2.6
1	D	313	ALA	2.6
1	B	311	ASP	2.6
1	E	164	SER	2.5
1	D	181	HIS	2.4
1	B	162	ASN	2.3
1	D	145	HIS	2.3
1	B	384	TYR	2.3
1	D	380	GLU	2.3
1	B	0	VAL	2.3
1	D	169	SER	2.3
1	D	168	ALA	2.2
1	A	311	ASP	2.2
1	D	129	PRO	2.2
1	E	259	ASP	2.2
1	A	163	GLN	2.2
1	D	273	GLY	2.1
1	D	256	LYS	2.1
1	E	295	SER	2.1
1	D	292	THR	2.1
1	D	314	THR	2.1
1	A	181	HIS	2.1
1	E	31	VAL	2.1
1	E	256	LYS	2.1
1	E	314	THR	2.1
1	B	181	HIS	2.1
1	B	229	SER	2.1
1	D	263	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	312	VAL	2.1
1	D	381	ASP	2.0
1	E	105	SER	2.0
1	A	68	TYR	2.0
1	A	33	THR	2.0
1	E	168	ALA	2.0
1	A	145	HIS	2.0
1	E	266	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

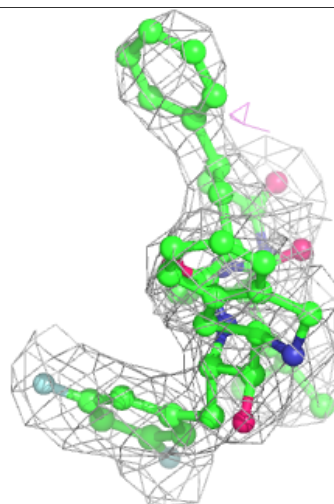
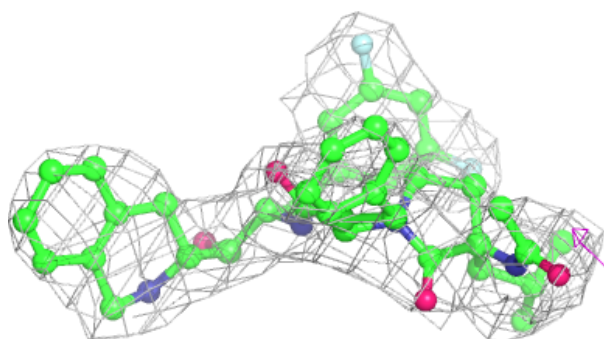
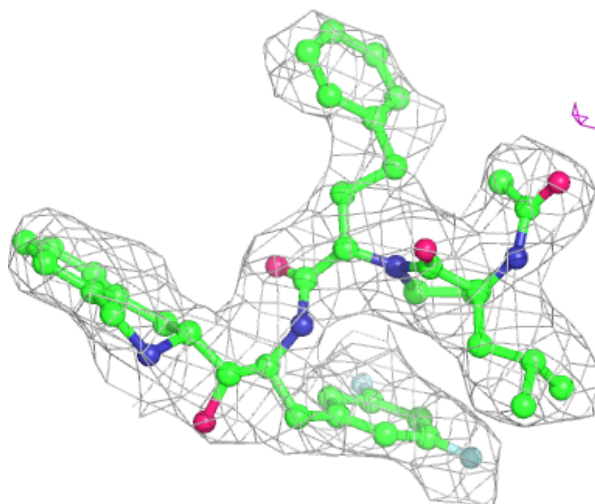
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PB8	E	394	48/48	0.91	0.21	6,15,20,22	0
2	PB8	D	394	48/48	0.93	0.18	3,15,24,25	0
2	PB8	B	394	48/48	0.93	0.19	3,10,15,20	0
2	PB8	A	394	48/48	0.94	0.19	2,11,21,24	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.

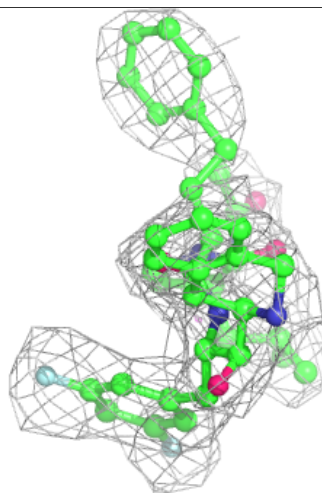
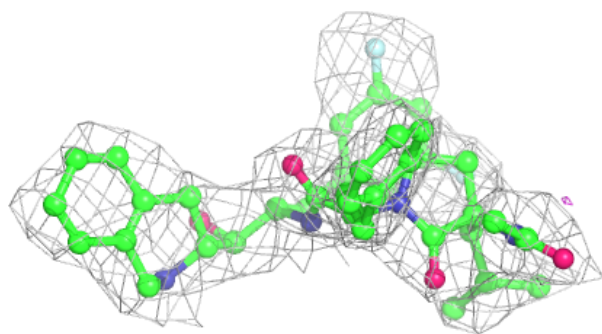
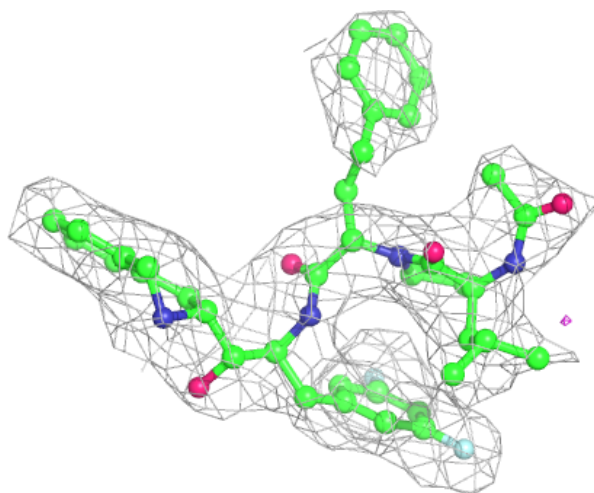
Electron density around PB8 E 394:

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



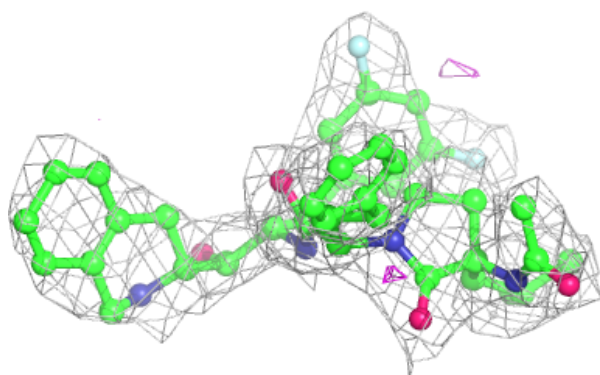
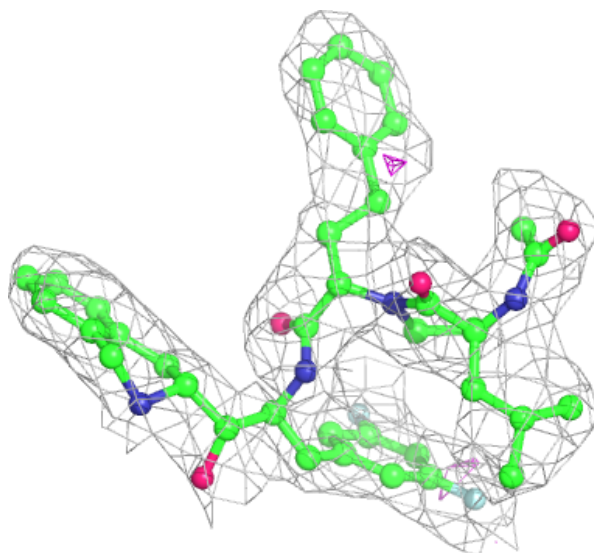
Electron density around PB8 D 394:

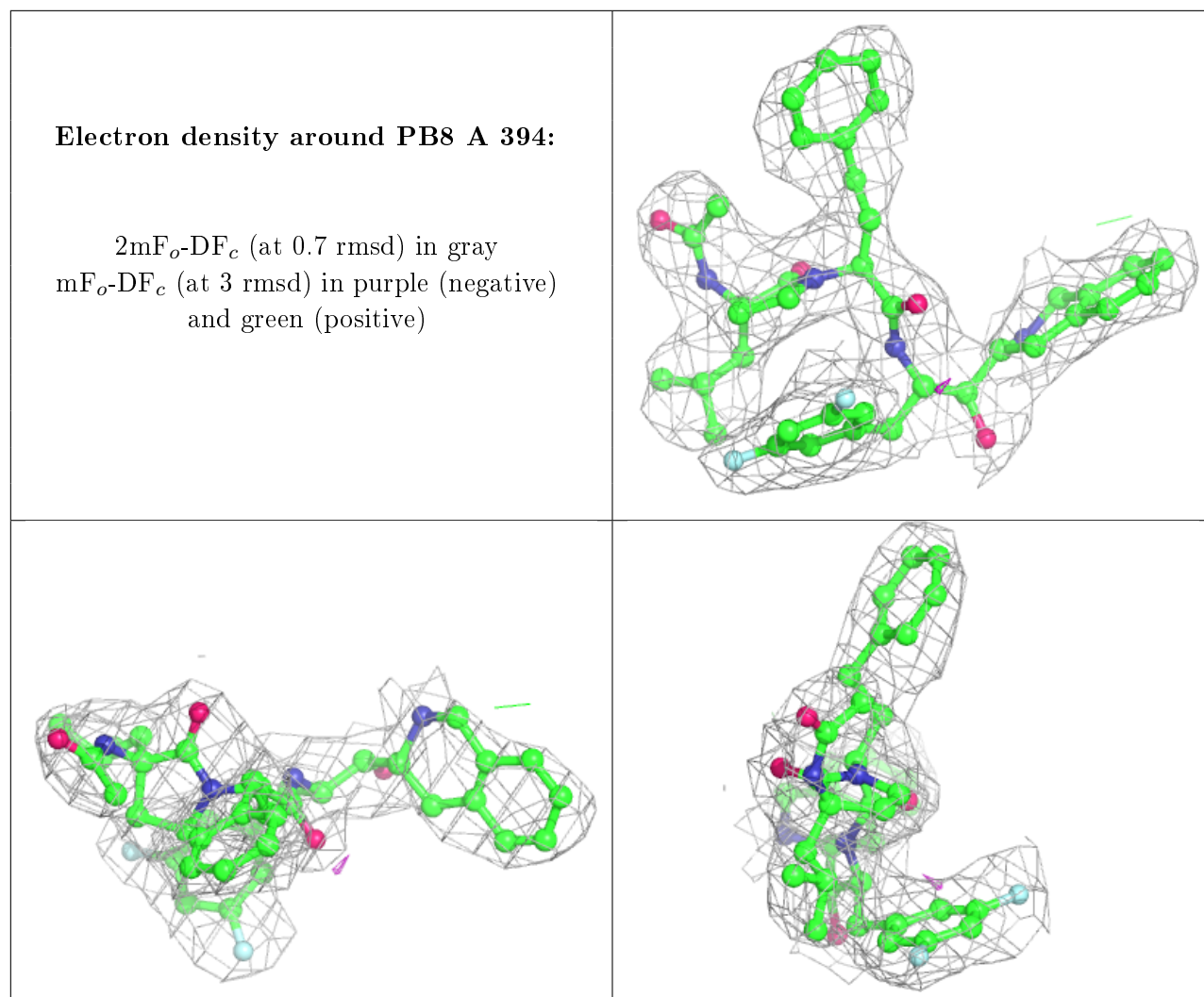
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PB8 B 394:

$2mF_o-DF_c$ (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.