



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 AM UTC

PDB ID : 3FAA / pdb_00003faa
Title : Crystal structure of TGFbRI complexed with a 2-aminoimidazole inhibitor
Authors : Boriack-Sjodin, P.A.; Fitch, C.
Deposited on : 2008-11-16
Resolution : 3.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

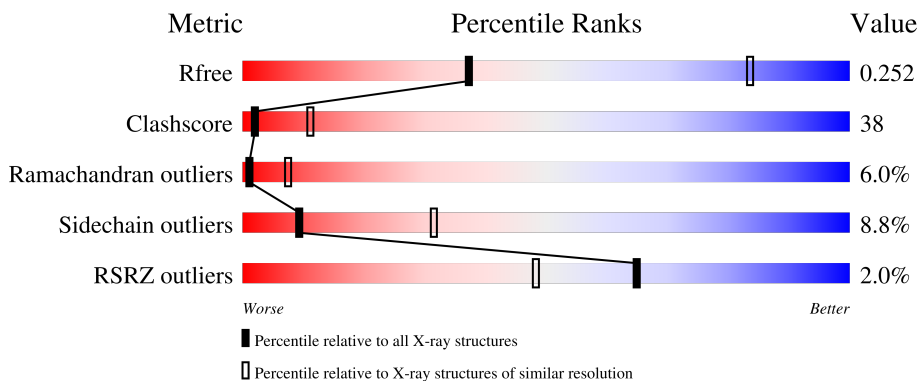
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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

Mol	Chain	Length	Quality of chain
1	A	342	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">39% 49% 8% . .</p>
1	B	342	<div style="display: flex; align-items: center;"> <div style="width: 46%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">46% 39% 10% . 5%</p>
1	C	342	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 57%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">28% 57% 10% . .</p>
1	D	342	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 41%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">41% 48% 7% .</p>
1	E	342	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">40% 45% 10% . .</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	9	-	-	X	-
3	PO4	D	13	-	-	X	-
3	PO4	E	2	-	-	X	-

2 Entry composition [i](#)

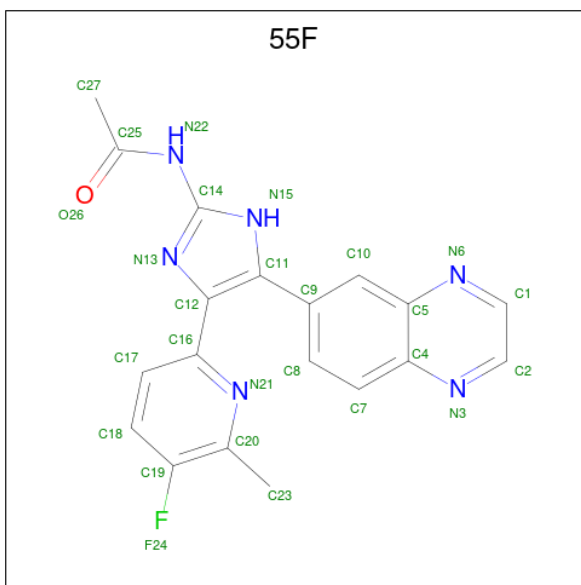
There are 3 unique types of molecules in this entry. The entry contains 13294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-beta receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	Total	C	N	O	S	0	0	0
			2617	1650	469	482	16			
1	B	324	Total	C	N	O	S	0	0	0
			2590	1636	463	475	16			
1	C	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	D	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	E	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			

- Molecule 2 is N-[4-(5-fluoro-6-methylpyridin-2-yl)-5-quinoxalin-6-yl-1H-imidazol-2-yl]acetamide (CCD ID: 55F) (formula: C₁₉H₁₅FN₆O).



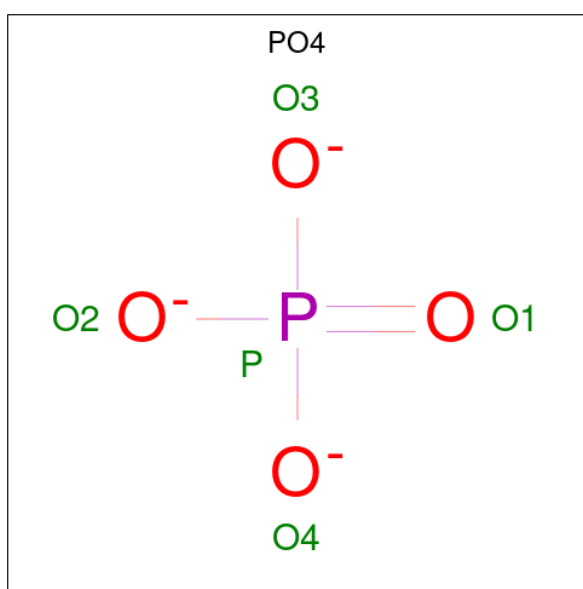
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	B	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	C	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	D	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	E	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O P	0	0
			5	4 1		
3	A	1	Total	O P	0	0
			5	4 1		
3	A	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	C	1	Total	O P	0	0
			5	4 1		

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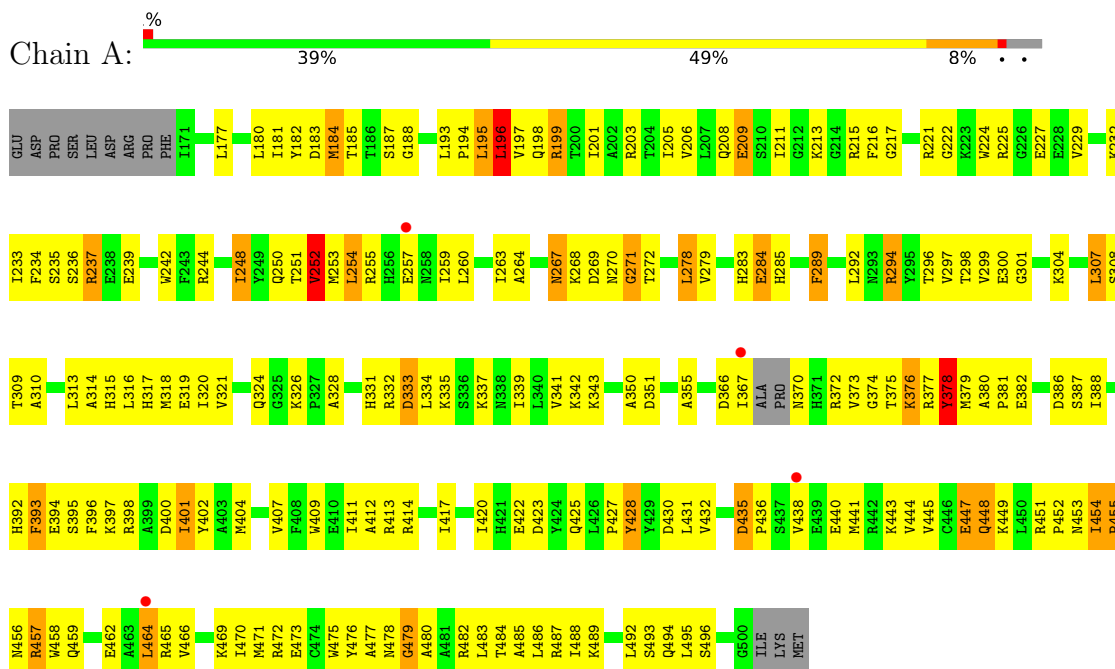
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

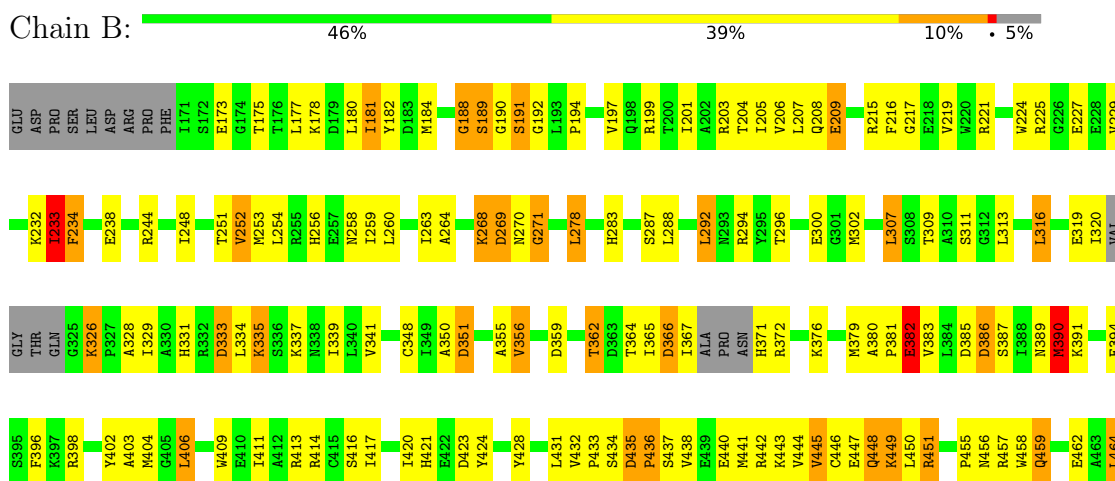
3 Residue-property plots i

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: TGF-beta receptor type-1

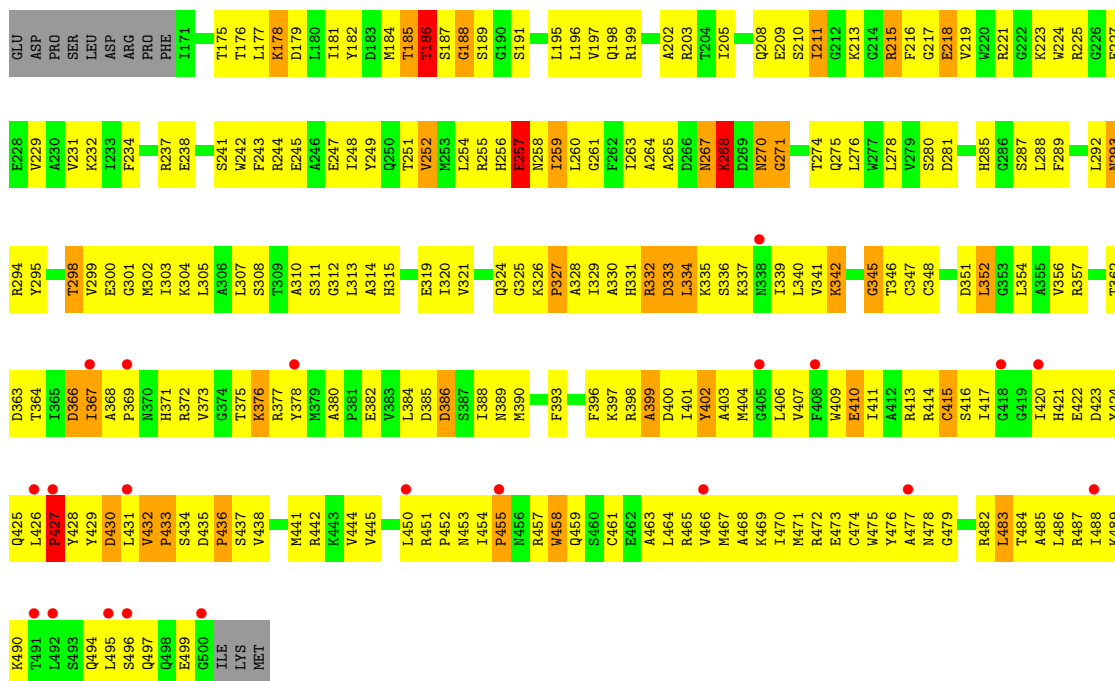


• Molecule 1: TGF-beta receptor type-1

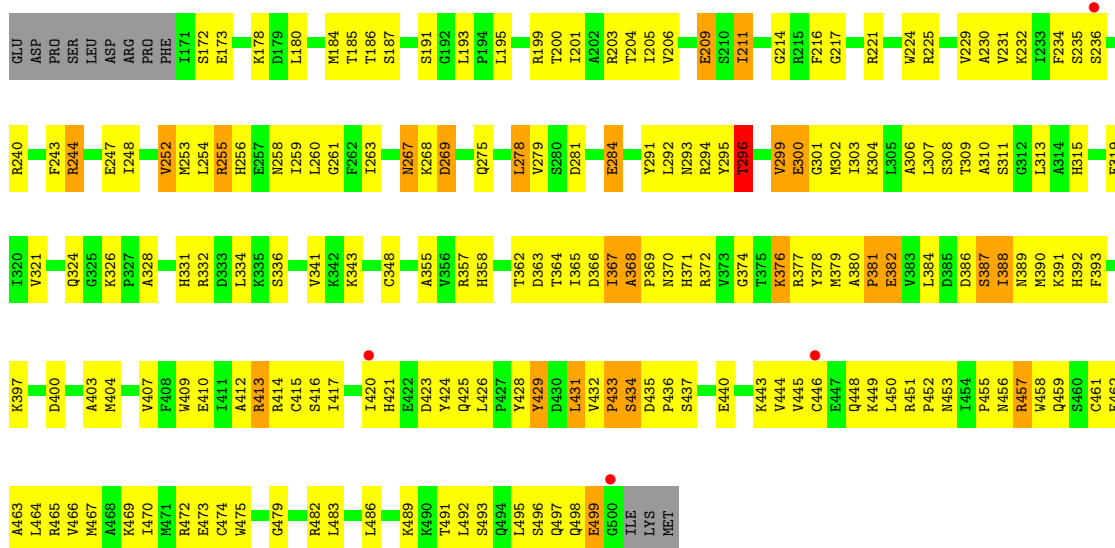




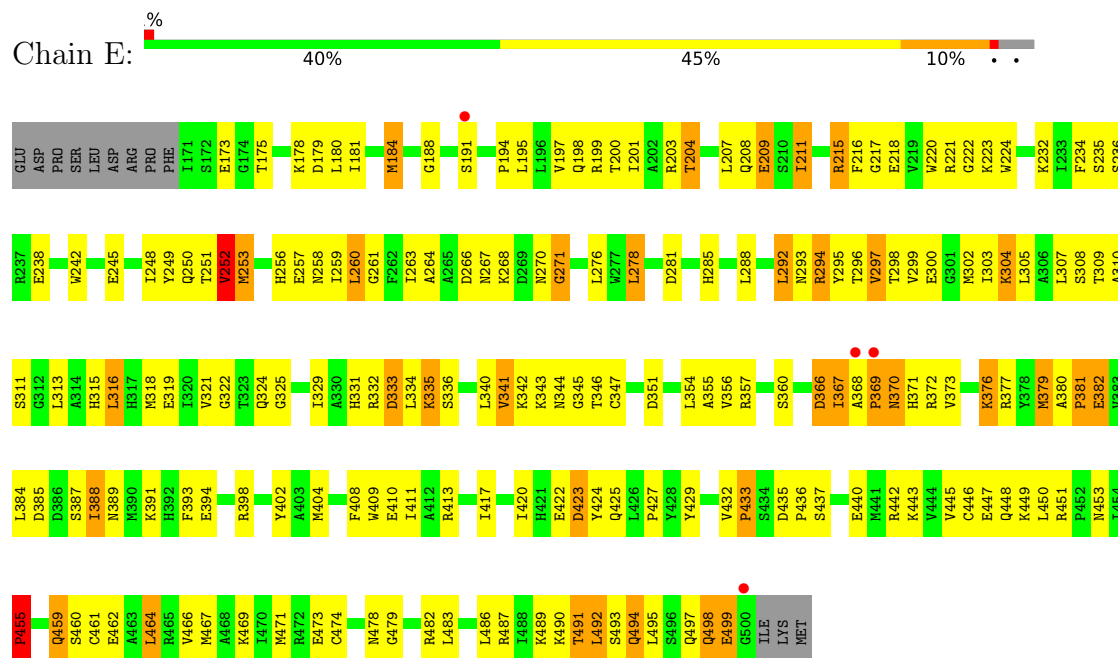
- Molecule 1: TGF-beta receptor type-1



- Molecule 1: TGF-beta receptor type-1



- Molecule 1: TGF-beta receptor type-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.86Å 248.85Å 138.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.35 35.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-3.35) 99.7 (35.00-3.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.19Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.271 0.206 , 0.252	Depositor DCC
R_{free} test set	2477 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13294	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 55F

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2668	0.96	10/3600 (0.3%)
1	B	0.57	0/2640	1.00	12/3560 (0.3%)
1	C	0.45	0/2682	0.98	8/3622 (0.2%)
1	D	0.54	0/2682	1.02	9/3622 (0.2%)
1	E	0.60	0/2682	1.06	12/3622 (0.3%)
All	All	0.53	0/13354	1.00	51/18026 (0.3%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASP	CA-C-N	7.37	127.28	120.21
1	A	435	ASP	C-N-CA	7.37	127.28	120.21
1	D	434	SER	N-CA-C	-7.20	98.99	110.14
1	A	248	ILE	N-CA-C	7.15	117.14	110.42
1	B	268	LYS	N-CA-C	7.01	121.79	111.34
1	E	459	GLN	N-CA-C	-6.88	105.82	114.56
1	A	268	LYS	N-CA-C	6.88	125.44	110.80
1	D	284	GLU	N-CA-C	6.50	119.20	111.33
1	E	297	VAL	N-CA-C	6.50	117.71	108.42
1	C	410	GLU	N-CA-C	-6.41	105.28	113.23
1	E	268	LYS	N-CA-C	6.33	124.27	110.80
1	E	494	GLN	N-CA-C	-6.26	103.60	111.11
1	D	299	VAL	N-CA-C	-6.20	104.46	110.72
1	D	387	SER	N-CA-C	-6.17	104.98	113.18
1	E	266	ASP	N-CA-C	6.16	118.42	108.32
1	E	370	ASN	N-CA-C	5.96	118.57	109.62
1	B	445	VAL	N-CA-C	5.95	116.59	110.82
1	B	296	THR	N-CA-C	-5.88	100.11	109.23
1	E	474	CYS	N-CA-C	-5.85	105.99	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ILE	N-CA-C	5.83	115.95	110.30
1	B	435	ASP	CA-C-N	5.83	127.13	119.84
1	B	435	ASP	C-N-CA	5.83	127.13	119.84
1	E	492	LEU	N-CA-C	-5.80	106.05	113.01
1	E	252	VAL	N-CA-C	5.80	121.40	109.34
1	A	472	ARG	N-CA-C	-5.74	106.12	113.23
1	B	459	GLN	N-CA-C	-5.71	106.66	113.97
1	A	252	VAL	N-CA-C	5.62	121.04	109.34
1	C	293	ASN	N-CA-C	-5.62	105.56	113.20
1	C	268	LYS	N-CA-C	5.49	122.48	110.80
1	E	437	SER	N-CA-C	-5.48	101.23	109.95
1	A	233	ILE	N-CA-C	5.47	114.62	106.85
1	C	371	HIS	N-CA-C	-5.46	102.43	110.52
1	D	172	SER	N-CA-C	5.45	117.57	110.43
1	B	233	ILE	N-CA-C	5.43	115.92	107.99
1	A	285	HIS	N-CA-C	5.42	118.68	111.75
1	D	296	THR	N-CA-C	-5.35	101.04	109.50
1	D	368	ALA	CA-C-N	5.34	126.52	119.84
1	D	368	ALA	C-N-CA	5.34	126.52	119.84
1	D	370	ASN	N-CA-C	-5.27	106.16	112.59
1	C	270	ASN	N-CA-C	5.22	117.46	109.95
1	C	499	GLU	N-CA-C	-5.19	108.21	114.75
1	B	498	GLN	N-CA-C	-5.16	105.66	111.28
1	A	314	ALA	N-CA-C	-5.16	105.31	111.03
1	B	181	ILE	N-CA-C	5.16	115.38	110.53
1	E	296	THR	N-CA-C	-5.14	101.63	109.65
1	C	252	VAL	N-CA-C	5.11	119.97	109.34
1	B	219	VAL	N-CA-C	-5.09	101.14	108.53
1	E	321	VAL	N-CA-C	5.08	119.15	112.04
1	B	326	LYS	CA-C-N	5.05	125.03	120.03
1	B	326	LYS	C-N-CA	5.05	125.03	120.03
1	C	231	VAL	N-CA-C	5.02	115.27	107.28

There are no chirality outliers.

There are no planarity outliers.

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	2617	0	2618	207	0
1	B	2590	0	2595	167	0
1	C	2629	0	2631	286	0
1	D	2629	0	2631	177	0
1	E	2629	0	2631	187	0
2	A	27	0	15	1	0
2	B	27	0	15	2	0
2	C	27	0	15	1	0
2	D	27	0	15	0	0
2	E	27	0	15	1	0
3	A	15	0	0	2	0
3	B	15	0	0	1	0
3	C	5	0	0	0	0
3	D	15	0	0	2	0
3	E	15	0	0	2	0
All	All	13294	0	13181	1012	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 38.

All (1012) 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:D:417:ILE:HD11	1:D:457:ARG:HH12	1.08	1.11
1:D:184:MET:HE3	1:D:193:LEU:HG	1.30	1.05
1:E:367:ILE:HD13	1:E:370:ASN:HD21	1.21	1.02
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.39	1.02
1:A:417:ILE:HD11	1:A:457:ARG:HH12	1.26	0.99
1:E:256:HIS:HD2	1:E:258:ASN:H	0.99	0.98
1:C:298:THR:HG22	1:C:300:GLU:H	1.28	0.97
1:A:309:THR:HG22	1:A:404:MET:HE2	1.46	0.96
1:A:376:LYS:HE3	1:A:438:VAL:HG13	1.49	0.94
1:D:253:MET:HB2	1:D:326:LYS:HB2	1.50	0.94
1:B:376:LYS:HA	1:B:379:MET:HE3	1.49	0.93
1:E:487:ARG:HH21	1:E:490:LYS:HD2	1.35	0.92
1:C:216:PHE:HD1	1:C:217:GLY:N	1.67	0.91
1:B:406:LEU:HD12	1:B:406:LEU:H	1.34	0.90
1:D:368:ALA:HB2	1:E:178:LYS:HE3	1.52	0.90
1:C:267:ASN:HD22	1:C:267:ASN:H	1.14	0.89
1:A:298:THR:HG22	1:A:300:GLU:H	1.38	0.89
1:B:389:ASN:HD21	1:B:391:LYS:HD3	1.37	0.88
1:E:367:ILE:CD1	1:E:370:ASN:HD21	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:THR:HG22	1:B:404:MET:HE2	1.56	0.85
1:A:267:ASN:HD22	1:A:267:ASN:H	1.20	0.84
1:E:256:HIS:CD2	1:E:258:ASN:H	1.90	0.84
1:B:443:LYS:HG2	1:B:448:GLN:HE21	1.43	0.83
1:B:403:ALA:HA	1:B:406:LEU:HD13	1.58	0.83
1:C:216:PHE:CD1	1:C:217:GLY:N	2.46	0.83
1:C:417:ILE:HD13	1:C:461:CYS:SG	2.19	0.83
1:C:436:PRO:HB3	1:C:441:MET:SD	2.18	0.83
1:D:417:ILE:HD11	1:D:457:ARG:NH1	1.93	0.82
1:D:310:ALA:HA	1:D:404:MET:HE1	1.59	0.82
1:B:252:VAL:HG23	1:B:253:MET:H	1.44	0.82
1:E:256:HIS:HD2	1:E:258:ASN:N	1.78	0.81
1:A:388:ILE:HD11	1:A:395:SER:HB3	1.62	0.81
1:B:311:SER:HA	1:B:489:LYS:HG3	1.63	0.81
1:B:458:TRP:HZ3	1:B:471:MET:HE1	1.46	0.81
1:E:367:ILE:HD13	1:E:370:ASN:ND2	1.95	0.80
1:C:461:CYS:HB2	1:C:464:LEU:HD23	1.62	0.80
1:B:252:VAL:HG21	1:B:326:LYS:HA	1.63	0.79
1:C:368:ALA:N	1:C:369:PRO:HD2	1.98	0.79
1:A:443:LYS:HE2	1:A:448:GLN:NE2	1.98	0.79
1:C:335:LYS:CG	1:C:336:SER:H	1.96	0.79
1:A:216:PHE:HE2	1:A:232:LYS:HG3	1.48	0.79
1:A:413:ARG:HG2	1:A:413:ARG:HH11	1.47	0.79
1:B:199:ARG:HD2	1:B:203:ARG:NH1	1.98	0.79
1:D:252:VAL:HG23	1:D:253:MET:H	1.47	0.78
1:C:267:ASN:H	1:C:267:ASN:ND2	1.78	0.78
1:C:417:ILE:O	1:C:420:ILE:HG12	1.84	0.78
1:E:310:ALA:HA	1:E:404:MET:HE1	1.64	0.78
1:C:202:ALA:HA	1:C:205:ILE:HD12	1.65	0.77
1:A:470:ILE:HA	1:A:473:GLU:HB2	1.65	0.76
1:E:309:THR:HG22	1:E:404:MET:HE3	1.65	0.76
1:A:417:ILE:HD11	1:A:457:ARG:NH1	2.01	0.76
1:D:457:ARG:NH1	1:D:457:ARG:HB2	1.99	0.76
1:B:409:TRP:HA	1:B:471:MET:HE3	1.67	0.76
1:C:372:ARG:NH2	1:C:438:VAL:HG21	2.01	0.76
1:A:267:ASN:HD22	1:A:267:ASN:N	1.80	0.75
1:C:367:ILE:HG23	1:C:369:PRO:HG2	1.65	0.75
1:A:224:TRP:CH2	1:A:225:ARG:HD2	2.20	0.75
1:C:332:ARG:HB3	1:C:332:ARG:NH1	2.02	0.74
1:B:309:THR:HG22	1:B:404:MET:CE	2.17	0.74
1:A:469:LYS:HE2	1:A:473:GLU:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:HIS:HB3	1:C:259:ILE:HG13	1.69	0.74
1:E:368:ALA:HB3	1:E:369:PRO:HD3	1.68	0.74
1:C:444:VAL:HG13	1:C:450:LEU:HD12	1.70	0.74
1:C:487:ARG:NH2	1:C:490:LYS:HD2	2.02	0.74
1:D:433:PRO:HG2	1:D:440:GLU:OE2	1.87	0.74
1:E:310:ALA:CA	1:E:404:MET:HE1	2.17	0.73
1:E:377:ARG:HH12	3:E:2:PO4:P	2.11	0.73
1:A:428:TYR:HE2	1:A:445:VAL:HG22	1.53	0.73
1:C:302:MET:HG3	1:C:411:ILE:HG22	1.69	0.73
1:A:453:ASN:O	1:A:455:PRO:HD3	1.89	0.73
1:C:454:ILE:HD11	1:C:475:TRP:CZ3	2.23	0.73
1:C:215:ARG:HE	1:C:215:ARG:N	1.87	0.73
1:C:410:GLU:HB3	1:C:424:TYR:HE1	1.52	0.73
1:C:435:ASP:N	1:C:436:PRO:HD3	2.03	0.73
1:B:376:LYS:H	1:B:376:LYS:HD2	1.54	0.72
1:C:414:ARG:HD3	1:C:424:TYR:N	2.04	0.72
1:D:372:ARG:HD3	1:D:379:MET:SD	2.30	0.72
1:B:458:TRP:CZ3	1:B:471:MET:HE1	2.24	0.72
1:A:466:VAL:HG21	1:A:495:LEU:HD22	1.72	0.72
1:A:319:GLU:HB2	1:A:328:ALA:HB2	1.72	0.71
1:C:299:VAL:HG22	1:C:415:CYS:SG	2.30	0.71
1:C:302:MET:HE3	1:C:467:MET:HE2	1.71	0.71
1:C:479:GLY:HA2	1:C:482:ARG:HD2	1.72	0.71
1:E:487:ARG:O	1:E:491:THR:HG23	1.90	0.71
1:A:289:PHE:CD2	1:A:337:LYS:HE2	2.24	0.71
1:B:233:ILE:HD13	1:B:233:ILE:O	1.90	0.71
1:B:201:ILE:O	1:B:205:ILE:HG13	1.90	0.71
1:E:487:ARG:HH21	1:E:490:LYS:CD	2.02	0.71
1:C:307:LEU:HD23	1:C:307:LEU:O	1.90	0.71
1:D:462:GLU:O	1:D:466:VAL:HG23	1.90	0.71
1:C:181:ILE:O	1:C:185:THR:HG22	1.91	0.70
1:A:380:ALA:HA	1:A:402:TYR:CE1	2.27	0.70
1:C:335:LYS:HG3	1:C:336:SER:H	1.55	0.70
1:C:335:LYS:CG	1:C:336:SER:N	2.54	0.70
1:E:303:ILE:HD13	1:E:495:LEU:HG	1.73	0.70
1:A:466:VAL:O	1:A:470:ILE:HG13	1.92	0.70
1:E:313:LEU:HD13	1:E:334:LEU:HD11	1.74	0.70
1:C:384:LEU:HD22	1:C:442:ARG:HB2	1.73	0.70
1:C:409:TRP:HB2	1:C:471:MET:HE3	1.74	0.70
1:A:459:GLN:OE1	1:A:465:ARG:HG2	1.92	0.69
1:D:307:LEU:HA	1:D:492:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:GLN:O	1:D:497:GLN:HG2	1.91	0.69
1:C:332:ARG:HB3	1:C:332:ARG:HH11	1.57	0.69
1:C:459:GLN:HE22	1:C:465:ARG:HG3	1.56	0.69
1:B:406:LEU:HD12	1:B:406:LEU:N	2.08	0.69
1:E:459:GLN:HA	1:E:459:GLN:NE2	2.05	0.69
1:E:459:GLN:HA	1:E:459:GLN:HE21	1.58	0.69
1:C:256:HIS:HB3	1:C:259:ILE:CD1	2.22	0.69
1:D:315:HIS:O	1:D:326:LYS:HE3	1.92	0.69
1:D:431:LEU:HD22	1:D:444:VAL:HG13	1.75	0.69
1:C:413:ARG:HD3	1:C:423:ASP:O	1.94	0.68
1:B:406:LEU:H	1:B:406:LEU:CD1	2.06	0.68
1:C:377:ARG:HA	1:C:441:MET:HE2	1.74	0.68
1:C:469:LYS:O	1:C:473:GLU:HG3	1.93	0.68
1:E:332:ARG:HH22	1:E:369:PRO:HG2	1.58	0.68
1:B:450:LEU:O	1:B:451:ARG:HD3	1.94	0.68
1:E:298:THR:HG22	1:E:299:VAL:N	2.10	0.67
1:C:398:ARG:HB3	1:C:482:ARG:HH11	1.59	0.67
1:E:253:MET:HE2	1:E:325:GLY:HA2	1.76	0.67
1:C:267:ASN:ND2	1:C:267:ASN:N	2.37	0.67
1:C:483:LEU:HD13	1:C:488:ILE:HD11	1.77	0.67
1:A:313:LEU:HD11	1:A:317:HIS:HE2	1.58	0.67
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.76	0.67
1:C:258:ASN:O	1:C:348:CYS:HA	1.94	0.67
1:B:493:SER:O	1:B:496:SER:HB3	1.95	0.67
1:E:490:LYS:O	1:E:493:SER:HB2	1.94	0.67
1:D:417:ILE:HG13	1:D:420:ILE:HG13	1.77	0.67
1:E:204:THR:HG22	1:E:224:TRP:NE1	2.09	0.67
1:B:178:LYS:HD2	1:B:227:GLU:OE2	1.95	0.67
1:D:469:LYS:O	1:D:473:GLU:HG2	1.95	0.66
1:A:317:HIS:HB3	1:A:397:LYS:HE2	1.76	0.66
1:C:285:HIS:HD2	1:C:342:LYS:O	1.79	0.66
1:C:372:ARG:HH12	1:C:438:VAL:HG11	1.61	0.66
1:C:232:LYS:HD2	1:C:234:PHE:CZ	2.30	0.66
1:C:420:ILE:HG13	1:C:420:ILE:O	1.94	0.66
1:A:469:LYS:HE2	1:A:473:GLU:CG	2.26	0.66
1:C:256:HIS:HB3	1:C:259:ILE:CG1	2.26	0.66
1:D:216:PHE:CD1	1:D:217:GLY:N	2.64	0.65
1:E:334:LEU:O	1:E:335:LYS:HB3	1.96	0.65
1:E:298:THR:HG22	1:E:300:GLU:H	1.61	0.65
1:A:267:ASN:N	1:A:267:ASN:ND2	2.41	0.65
1:C:268:LYS:HB2	1:C:275:GLN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ILE:HB	1:D:279:VAL:HG12	1.78	0.65
1:E:181:ILE:HA	1:E:184:MET:HE3	1.77	0.65
1:A:309:THR:HG22	1:A:404:MET:CE	2.25	0.65
1:E:198:GLN:HE22	1:E:250:GLN:HE22	1.45	0.65
1:B:376:LYS:HA	1:B:379:MET:CE	2.25	0.64
1:C:434:SER:C	1:C:436:PRO:HD3	2.22	0.64
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.28	0.64
1:B:248:ILE:CD1	1:B:355:ALA:HB3	2.28	0.64
1:D:294:ARG:HD3	1:D:295:TYR:CE2	2.31	0.64
1:E:331:HIS:O	1:E:332:ARG:HB2	1.97	0.64
1:E:245:GLU:HG2	1:E:249:TYR:HE1	1.63	0.64
1:C:453:ASN:O	1:C:455:PRO:HD3	1.97	0.64
1:D:466:VAL:O	1:D:469:LYS:HB3	1.98	0.64
1:C:334:LEU:HD23	1:C:335:LYS:N	2.13	0.63
1:C:254:LEU:HD11	1:C:259:ILE:HG21	1.80	0.63
1:C:320:ILE:HG22	1:C:321:VAL:N	2.13	0.63
1:C:474:CYS:SG	1:C:483:LEU:HD11	2.38	0.63
1:D:209:GLU:OE2	1:D:221:ARG:NH1	2.29	0.63
1:D:254:LEU:HD11	1:D:259:ILE:HG21	1.80	0.63
1:C:334:LEU:HD23	1:C:335:LYS:H	1.62	0.63
1:C:473:GLU:HA	1:C:476:TYR:CZ	2.32	0.63
1:D:457:ARG:CB	1:D:457:ARG:HH11	2.12	0.63
1:C:473:GLU:HB3	1:C:483:LEU:HG	1.80	0.63
1:B:381:PRO:HD2	1:B:482:ARG:HH22	1.63	0.63
1:C:413:ARG:HG3	1:C:422:GLU:HB2	1.81	0.63
1:A:486:LEU:O	1:A:489:LYS:HB3	1.99	0.63
1:D:178:LYS:HD2	1:D:178:LYS:N	2.13	0.63
1:D:451:ARG:HG2	1:D:475:TRP:HB3	1.80	0.63
1:C:410:GLU:HB3	1:C:424:TYR:CE1	2.33	0.63
1:A:476:TYR:C	1:A:478:ASN:H	2.07	0.62
1:B:414:ARG:HD2	1:B:424:TYR:HB2	1.81	0.62
1:D:229:VAL:HG11	1:D:279:VAL:HG13	1.81	0.62
1:A:208:GLN:HG2	1:A:222:GLY:HA2	1.79	0.62
1:A:428:TYR:CE2	1:A:445:VAL:HG22	2.35	0.62
1:A:248:ILE:HA	1:A:251:THR:HG23	1.82	0.62
1:C:377:ARG:HE	1:C:436:PRO:HG2	1.64	0.62
1:E:318:MET:HG2	1:E:319:GLU:N	2.15	0.62
1:E:367:ILE:CG1	1:E:370:ASN:HD21	2.12	0.62
1:C:384:LEU:HD13	1:C:442:ARG:HA	1.79	0.62
1:D:457:ARG:NH1	1:D:457:ARG:CB	2.62	0.62
1:A:267:ASN:H	1:A:267:ASN:ND2	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:TYR:HD1	1:A:378:TYR:H	1.46	0.62
1:A:398:ARG:CZ	1:A:480:ALA:HA	2.30	0.62
1:C:305:LEU:HD13	1:C:305:LEU:O	1.99	0.62
1:C:398:ARG:HD3	1:C:479:GLY:HA3	1.82	0.62
1:A:199:ARG:HD2	1:A:203:ARG:CZ	2.30	0.61
1:C:303:ILE:O	1:C:307:LEU:HB2	2.00	0.61
1:D:216:PHE:CG	1:D:217:GLY:N	2.68	0.61
1:E:259:ILE:O	1:E:260:LEU:C	2.42	0.61
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.65	0.61
1:B:479:GLY:HA2	1:B:482:ARG:HD2	1.82	0.61
1:B:319:GLU:HB2	1:B:328:ALA:HB2	1.82	0.61
1:B:334:LEU:O	1:B:335:LYS:HB3	1.99	0.61
1:D:368:ALA:HB2	1:E:178:LYS:CE	2.29	0.61
1:D:382:GLU:CD	1:D:482:ARG:HH22	2.08	0.61
1:A:380:ALA:HA	1:A:402:TYR:CD1	2.36	0.61
1:B:316:LEU:HD22	1:B:329:ILE:HB	1.82	0.61
1:D:431:LEU:HD11	1:D:450:LEU:HD13	1.81	0.61
1:A:248:ILE:O	1:A:251:THR:HG23	2.00	0.61
1:A:294:ARG:O	1:A:294:ARG:HD3	2.01	0.61
1:B:199:ARG:HD2	1:B:203:ARG:CZ	2.31	0.61
1:D:243:PHE:CZ	1:E:175:THR:HG23	2.35	0.61
1:E:433:PRO:HG2	1:E:440:GLU:OE2	2.01	0.61
1:D:252:VAL:HG23	1:D:253:MET:N	2.16	0.61
1:A:367:ILE:HD12	1:A:370:ASN:HB2	1.83	0.61
1:C:258:ASN:OD1	1:C:308:SER:HB2	2.01	0.61
1:C:461:CYS:CB	1:C:464:LEU:HD23	2.29	0.61
1:C:495:LEU:O	1:C:495:LEU:HG	2.01	0.61
1:D:296:THR:HG21	1:D:421:HIS:CD2	2.35	0.61
1:D:437:SER:OG	1:D:440:GLU:HG3	2.01	0.61
1:A:211:ILE:HD12	1:A:211:ILE:O	2.01	0.60
1:C:384:LEU:HD23	1:C:438:VAL:HG13	1.81	0.60
1:D:413:ARG:O	1:D:414:ARG:HG2	2.01	0.60
1:E:200:THR:O	1:E:204:THR:HB	2.01	0.60
1:C:377:ARG:CG	1:C:436:PRO:HG2	2.31	0.60
1:B:184:MET:HE3	1:B:191:SER:O	2.00	0.60
1:C:414:ARG:HD3	1:C:424:TYR:H	1.65	0.60
1:E:497:GLN:C	1:E:499:GLU:H	2.09	0.60
1:B:409:TRP:CA	1:B:471:MET:HE3	2.29	0.60
1:C:217:GLY:O	1:C:218:GLU:HB2	2.02	0.60
1:C:397:LYS:O	1:C:401:ILE:HG12	2.01	0.60
1:C:351:ASP:C	1:C:352:LEU:HD23	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:VAL:O	1:C:470:ILE:HG13	2.01	0.60
1:C:479:GLY:HA2	1:C:482:ARG:CD	2.32	0.60
1:D:343:LYS:HB2	3:D:13:PO4:O4	2.02	0.60
1:D:498:GLN:O	1:D:499:GLU:HG3	2.01	0.60
1:E:253:MET:HE2	1:E:324:GLN:O	2.02	0.60
1:B:252:VAL:HG23	1:B:253:MET:N	2.16	0.60
1:E:356:VAL:HG23	1:E:393:PHE:HE1	1.66	0.60
1:B:362:THR:O	1:B:364:THR:HG23	2.02	0.60
1:C:287:SER:HB2	1:C:337:LYS:HA	1.84	0.59
1:C:352:LEU:HD23	1:C:352:LEU:N	2.16	0.59
1:A:289:PHE:CE2	1:A:337:LYS:HE2	2.38	0.59
1:A:377:ARG:C	1:A:379:MET:H	2.10	0.59
1:A:473:GLU:CD	1:A:483:LEU:HD21	2.27	0.59
1:B:381:PRO:C	1:B:383:VAL:H	2.09	0.59
1:D:267:ASN:OD1	1:D:267:ASN:N	2.34	0.59
1:E:218:GLU:CD	1:E:220:TRP:HE1	2.10	0.59
1:C:471:MET:HE2	1:C:475:TRP:CH2	2.37	0.59
1:D:469:LYS:HD2	1:D:472:ARG:HH21	1.67	0.59
1:A:209:GLU:OE2	1:A:221:ARG:NH1	2.31	0.59
1:A:216:PHE:CE2	1:A:232:LYS:HG3	2.33	0.59
1:B:178:LYS:HG2	1:C:368:ALA:HB3	1.85	0.59
1:B:376:LYS:HD2	1:B:376:LYS:N	2.18	0.59
1:C:335:LYS:HG2	1:C:336:SER:N	2.17	0.59
1:C:372:ARG:NH1	1:C:438:VAL:HG11	2.16	0.59
1:E:204:THR:CG2	1:E:224:TRP:HE1	2.16	0.59
1:C:261:GLY:HA3	1:C:281:ASP:OD2	2.02	0.59
1:E:413:ARG:NH1	1:E:423:ASP:O	2.36	0.59
1:D:378:TYR:OH	1:D:410:GLU:OE2	2.19	0.58
1:A:310:ALA:HA	1:A:404:MET:HE1	1.85	0.58
1:B:359:ASP:OD2	1:B:362:THR:HG23	2.03	0.58
1:C:292:LEU:C	1:C:294:ARG:H	2.11	0.58
1:D:205:ILE:CG2	1:D:206:VAL:N	2.65	0.58
1:E:447:GLU:O	1:E:449:LYS:HG3	2.04	0.58
1:B:251:THR:HG23	1:B:252:VAL:HG22	1.86	0.58
1:C:385:ASP:HA	1:C:442:ARG:CD	2.33	0.58
1:D:205:ILE:HG22	1:D:206:VAL:N	2.16	0.58
1:E:425:GLN:OE1	1:E:429:TYR:CD1	2.56	0.58
1:B:302:MET:CE	1:B:467:MET:HG3	2.33	0.58
1:C:357:ARG:HB2	1:C:366:ASP:HB2	1.85	0.58
1:E:332:ARG:NH2	1:E:369:PRO:HG2	2.18	0.58
1:E:404:MET:HE2	1:E:408:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD13	1:A:444:VAL:HG11	1.86	0.58
1:C:382:GLU:H	1:C:382:GLU:CD	2.12	0.58
1:D:389:ASN:ND2	1:D:391:LYS:H	2.02	0.58
1:A:409:TRP:HD1	1:A:471:MET:HE1	1.68	0.58
1:B:365:ILE:HG13	1:B:367:ILE:HB	1.85	0.58
1:E:469:LYS:HG3	1:E:473:GLU:OE2	2.03	0.58
1:C:368:ALA:N	1:C:369:PRO:CD	2.66	0.58
1:C:403:ALA:O	1:C:407:VAL:HG23	2.04	0.57
1:C:417:ILE:HD12	1:C:457:ARG:NH1	2.19	0.57
1:D:390:MET:HE2	1:D:390:MET:HA	1.85	0.57
1:E:367:ILE:HD12	1:E:367:ILE:N	2.20	0.57
1:C:382:GLU:HB3	1:C:388:ILE:HB	1.86	0.57
1:D:459:GLN:HE21	1:D:465:ARG:NH1	2.01	0.57
1:E:245:GLU:HG2	1:E:249:TYR:CE1	2.39	0.57
1:A:470:ILE:CD1	1:A:492:LEU:HD11	2.33	0.57
1:B:365:ILE:C	1:B:367:ILE:H	2.12	0.57
1:C:244:ARG:HH22	1:C:366:ASP:CG	2.12	0.57
1:D:293:ASN:ND2	1:D:424:TYR:CG	2.71	0.57
1:D:431:LEU:HD11	1:D:450:LEU:HD22	1.86	0.57
1:D:229:VAL:CG1	1:D:279:VAL:HG13	2.34	0.57
1:E:410:GLU:OE1	1:E:424:TYR:OH	2.22	0.57
1:C:308:SER:OG	1:C:347:CYS:HB2	2.04	0.57
1:D:362:THR:O	1:D:364:THR:HG23	2.05	0.57
1:D:498:GLN:O	1:D:499:GLU:CG	2.52	0.57
1:E:173:GLU:N	1:E:173:GLU:OE1	2.38	0.57
1:B:389:ASN:ND2	1:B:391:LYS:HD3	2.15	0.57
1:E:204:THR:HG22	1:E:224:TRP:CD1	2.40	0.57
1:E:245:GLU:HB3	1:E:278:LEU:HD21	1.87	0.57
1:C:256:HIS:HB3	1:C:259:ILE:HD11	1.86	0.57
1:D:299:VAL:HA	1:D:415:CYS:SG	2.44	0.57
1:D:466:VAL:HG21	1:D:495:LEU:HD22	1.87	0.57
1:B:437:SER:OG	1:B:440:GLU:HG3	2.05	0.57
1:C:260:LEU:HD13	1:C:340:LEU:HD12	1.87	0.57
1:D:311:SER:HA	1:D:489:LYS:HD2	1.87	0.57
1:D:431:LEU:CD1	1:D:450:LEU:HD13	2.35	0.57
1:E:389:ASN:ND2	1:E:391:LYS:HB3	2.19	0.57
1:E:487:ARG:NH2	1:E:490:LYS:HD2	2.14	0.57
1:A:184:MET:HE2	1:A:193:LEU:HG	1.86	0.56
1:C:406:LEU:HB3	1:C:427:PRO:HG2	1.87	0.56
1:D:307:LEU:CA	1:D:492:LEU:HD23	2.35	0.56
1:E:445:VAL:HG13	1:E:451:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:NH2	1:A:373:VAL:HG11	2.21	0.56
1:B:173:GLU:N	1:B:173:GLU:OE1	2.37	0.56
1:D:455:PRO:HD2	1:D:458:TRP:CZ3	2.40	0.56
1:D:456:ASN:O	1:D:459:GLN:HG2	2.05	0.56
1:B:390:MET:HE2	1:B:396:PHE:CE2	2.39	0.56
1:D:185:THR:C	1:D:187:SER:H	2.13	0.56
1:E:256:HIS:CD2	1:E:257:GLU:N	2.73	0.56
1:E:404:MET:HE2	1:E:408:PHE:CE2	2.41	0.56
1:B:367:ILE:HD11	1:B:371:HIS:CE1	2.40	0.56
1:C:451:ARG:HG2	1:C:475:TRP:HB3	1.87	0.56
1:A:407:VAL:O	1:A:411:ILE:HG13	2.05	0.56
1:E:308:SER:OG	1:E:346:THR:HG23	2.06	0.56
1:B:381:PRO:O	1:B:383:VAL:N	2.39	0.56
1:E:197:VAL:O	1:E:201:ILE:HG13	2.06	0.56
1:A:313:LEU:HD21	1:A:400:ASP:HB3	1.88	0.56
1:B:451:ARG:HE	1:B:475:TRP:HB3	1.70	0.56
1:C:199:ARG:O	1:C:203:ARG:HG3	2.05	0.56
1:A:473:GLU:HB3	1:A:483:LEU:HG	1.88	0.56
1:B:216:PHE:CD2	1:B:232:LYS:HE3	2.41	0.56
1:C:356:VAL:HG23	1:C:393:PHE:HE1	1.71	0.56
1:C:385:ASP:HA	1:C:442:ARG:HD2	1.87	0.56
1:D:367:ILE:CG1	1:D:369:PRO:HD3	2.24	0.56
1:E:409:TRP:CA	1:E:471:MET:HE3	2.35	0.56
1:C:430:ASP:OD1	1:C:431:LEU:HG	2.06	0.56
1:D:256:HIS:HD2	1:D:258:ASN:HB2	1.71	0.55
1:E:251:THR:O	1:E:253:MET:N	2.39	0.55
1:B:224:TRP:CH2	1:B:225:ARG:HD2	2.42	0.55
1:C:368:ALA:H	1:C:369:PRO:HD2	1.70	0.55
1:D:458:TRP:HB3	1:D:464:LEU:HB3	1.88	0.55
1:A:376:LYS:HE3	1:A:438:VAL:CG1	2.32	0.55
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.68	0.55
1:A:335:LYS:O	1:A:339:ILE:HG13	2.07	0.55
1:A:473:GLU:OE2	1:A:483:LEU:HD21	2.06	0.55
1:B:462:GLU:O	1:B:466:VAL:HG23	2.06	0.55
1:C:367:ILE:HG23	1:C:369:PRO:CG	2.35	0.55
1:C:407:VAL:HA	1:C:410:GLU:OE2	2.06	0.55
1:C:409:TRP:HB2	1:C:471:MET:CE	2.37	0.55
1:C:409:TRP:HD1	1:C:471:MET:HE1	1.71	0.55
1:A:413:ARG:HG2	1:A:413:ARG:NH1	2.16	0.55
1:A:470:ILE:HG23	1:A:483:LEU:HD12	1.88	0.55
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ILE:HD13	2:E:601:55F:C1	2.37	0.55
1:E:376:LYS:O	1:E:379:MET:HB2	2.07	0.55
1:B:351:ASP:OD1	2:B:601:55F:N22	2.39	0.55
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.35	0.55
1:A:234:PHE:CE1	1:A:278:LEU:HD22	2.42	0.55
1:A:301:GLY:HA2	1:A:304:LYS:NZ	2.22	0.55
1:A:451:ARG:HG2	1:A:475:TRP:HB3	1.89	0.55
1:C:184:MET:C	1:C:186:THR:H	2.14	0.55
1:C:385:ASP:HA	1:C:442:ARG:NE	2.22	0.55
1:E:209:GLU:OE1	1:E:221:ARG:HD3	2.06	0.55
1:C:213:LYS:HD3	1:C:218:GLU:HG3	1.87	0.55
1:C:409:TRP:HZ3	1:C:425:GLN:O	1.89	0.54
1:E:309:THR:CG2	1:E:404:MET:HE3	2.37	0.54
1:A:388:ILE:CD1	1:A:395:SER:HB3	2.36	0.54
1:B:313:LEU:O	1:B:313:LEU:HG	2.06	0.54
1:B:389:ASN:C	1:B:391:LYS:H	2.14	0.54
1:B:188:GLY:O	1:B:189:SER:HB2	2.06	0.54
1:C:402:TYR:CE1	1:C:406:LEU:HD11	2.41	0.54
1:C:486:LEU:HD13	1:C:486:LEU:O	2.07	0.54
1:D:376:LYS:HA	1:D:379:MET:HE3	1.89	0.54
1:E:253:MET:CE	1:E:325:GLY:HA2	2.37	0.54
1:A:378:TYR:N	1:A:378:TYR:CD1	2.76	0.54
1:C:211:ILE:HD12	1:C:221:ARG:HB2	1.90	0.54
1:E:432:VAL:HG22	1:E:433:PRO:HD2	1.88	0.54
1:A:462:GLU:O	1:A:466:VAL:HG23	2.07	0.54
1:B:253:MET:HE3	1:B:320:ILE:HD12	1.89	0.54
1:C:267:ASN:HD22	1:C:267:ASN:N	1.83	0.54
1:C:489:LYS:O	1:C:489:LYS:HD3	2.07	0.54
1:B:302:MET:HE3	1:B:467:MET:HG3	1.89	0.54
1:B:413:ARG:NH1	1:B:423:ASP:O	2.41	0.54
1:B:488:ILE:O	1:B:492:LEU:HB2	2.07	0.54
1:C:216:PHE:HB2	1:C:234:PHE:CD2	2.43	0.54
1:D:224:TRP:CH2	1:D:225:ARG:HD2	2.43	0.54
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.08	0.54
1:D:459:GLN:NE2	1:D:465:ARG:HH11	2.06	0.54
1:B:309:THR:CG2	1:B:404:MET:HE2	2.32	0.54
1:C:431:LEU:O	1:C:432:VAL:HB	2.07	0.54
1:C:441:MET:O	1:C:445:VAL:HG23	2.08	0.54
1:E:261:GLY:HA3	1:E:281:ASP:OD2	2.08	0.54
1:B:458:TRP:CD1	1:B:458:TRP:N	2.75	0.53
1:C:176:THR:O	1:C:179:ASP:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HA	1:C:441:MET:CE	2.38	0.53
1:C:417:ILE:HB	1:C:420:ILE:HG12	1.90	0.53
1:D:310:ALA:HA	1:D:404:MET:CE	2.34	0.53
1:E:443:LYS:HG3	1:E:447:GLU:OE1	2.08	0.53
1:A:301:GLY:HA2	1:A:304:LYS:HZ3	1.73	0.53
1:A:320:ILE:HG22	1:A:321:VAL:N	2.23	0.53
1:D:389:ASN:C	1:D:389:ASN:HD22	2.15	0.53
1:E:207:LEU:C	1:E:208:GLN:HE21	2.16	0.53
1:B:367:ILE:HG23	1:B:367:ILE:O	2.08	0.53
1:D:229:VAL:HG12	1:D:230:ALA:N	2.23	0.53
1:D:234:PHE:CE1	1:D:278:LEU:HD22	2.44	0.53
1:D:461:CYS:SG	1:D:464:LEU:HD23	2.48	0.53
1:E:432:VAL:CG2	1:E:433:PRO:HD2	2.38	0.53
1:A:381:PRO:HG3	1:A:445:VAL:HG12	1.91	0.53
1:B:385:ASP:O	1:B:386:ASP:C	2.51	0.53
1:C:377:ARG:HE	1:C:436:PRO:CG	2.21	0.53
1:C:473:GLU:CB	1:C:483:LEU:HG	2.38	0.53
1:A:456:ASN:C	1:A:458:TRP:H	2.17	0.53
1:C:332:ARG:HE	1:C:356:VAL:CG1	2.21	0.53
1:D:331:HIS:O	1:D:332:ARG:HB2	2.08	0.53
1:A:184:MET:O	1:A:187:SER:HB3	2.09	0.53
1:C:319:GLU:HB2	1:C:328:ALA:HB2	1.91	0.53
1:D:434:SER:O	1:D:435:ASP:C	2.50	0.53
1:E:357:ARG:HB2	1:E:366:ASP:OD2	2.08	0.53
1:A:451:ARG:HB3	1:A:475:TRP:CE3	2.44	0.53
1:C:330:ALA:HB3	1:C:356:VAL:HG22	1.90	0.53
1:D:204:THR:CG2	1:D:224:TRP:HE1	2.21	0.53
1:D:302:MET:CE	1:D:467:MET:HG3	2.39	0.53
1:A:252:VAL:HG23	1:A:253:MET:N	2.24	0.53
1:A:412:ALA:C	1:A:414:ARG:H	2.16	0.53
1:B:331:HIS:HD2	1:B:333:ASP:N	2.07	0.53
1:B:432:VAL:CG2	1:B:433:PRO:HD2	2.39	0.53
1:E:191:SER:HB3	1:E:252:VAL:HA	1.89	0.53
1:B:180:LEU:HD13	1:B:201:ILE:HD11	1.91	0.52
1:C:494:GLN:HG3	1:C:497:GLN:NE2	2.24	0.52
1:E:409:TRP:HA	1:E:471:MET:CE	2.39	0.52
1:A:397:LYS:O	1:A:400:ASP:HB2	2.09	0.52
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.73	0.52
1:C:454:ILE:HD12	1:C:472:ARG:CZ	2.40	0.52
1:B:204:THR:CG2	1:B:224:TRP:HE1	2.23	0.52
1:C:313:LEU:HD22	1:C:334:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ILE:HD11	1:E:464:LEU:HD23	1.91	0.52
1:C:332:ARG:HH12	1:C:373:VAL:HB	1.75	0.52
1:D:388:ILE:O	1:D:388:ILE:HG23	2.09	0.52
1:D:473:GLU:HB3	1:D:483:LEU:HG	1.91	0.52
1:A:409:TRP:CZ3	1:A:427:PRO:HA	2.45	0.52
1:B:180:LEU:CD1	1:B:201:ILE:HD11	2.39	0.52
1:E:346:THR:HG22	1:E:347:CYS:N	2.23	0.52
1:A:297:VAL:HG22	1:A:298:THR:N	2.25	0.52
1:D:178:LYS:HD2	1:D:178:LYS:H	1.75	0.52
1:D:451:ARG:CG	1:D:475:TRP:HB3	2.39	0.52
1:D:457:ARG:HB2	1:D:457:ARG:CZ	2.38	0.52
1:C:310:ALA:HA	1:C:404:MET:HE1	1.91	0.52
1:C:426:LEU:O	1:C:427:PRO:C	2.53	0.52
1:A:317:HIS:NE2	1:A:400:ASP:OD2	2.43	0.52
1:E:382:GLU:CD	1:E:482:ARG:HH12	2.17	0.52
1:B:389:ASN:C	1:B:391:LYS:N	2.67	0.52
1:B:462:GLU:HA	1:B:462:GLU:OE1	2.09	0.52
1:A:413:ARG:NH1	1:A:423:ASP:O	2.43	0.52
1:E:216:PHE:CD1	1:E:217:GLY:N	2.78	0.51
1:E:453:ASN:O	1:E:455:PRO:HD3	2.10	0.51
1:E:497:GLN:C	1:E:499:GLU:N	2.67	0.51
1:E:389:ASN:HD21	1:E:391:LYS:CB	2.22	0.51
1:B:248:ILE:HD13	1:B:355:ALA:HB3	1.92	0.51
1:C:182:TYR:O	1:C:186:THR:HB	2.10	0.51
1:E:432:VAL:O	1:E:433:PRO:O	2.28	0.51
1:B:216:PHE:CG	1:B:217:GLY:N	2.77	0.51
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.75	0.51
1:B:394:GLU:O	1:B:398:ARG:HG3	2.11	0.51
1:C:354:LEU:HD22	1:C:373:VAL:HG11	1.91	0.51
1:C:435:ASP:N	1:C:436:PRO:CD	2.72	0.51
1:D:466:VAL:O	1:D:470:ILE:HG13	2.11	0.51
1:E:208:GLN:HG2	1:E:222:GLY:HA2	1.92	0.51
1:A:313:LEU:HD11	1:A:317:HIS:NE2	2.25	0.51
1:C:472:ARG:C	1:C:474:CYS:H	2.18	0.51
1:E:285:HIS:HB3	1:E:341:VAL:CG2	2.41	0.51
1:E:417:ILE:O	1:E:420:ILE:HG12	2.10	0.51
1:A:470:ILE:HD11	1:A:492:LEU:HD11	1.93	0.51
1:D:416:SER:HA	1:D:421:HIS:HB3	1.93	0.51
1:E:256:HIS:ND1	1:E:315:HIS:CD2	2.79	0.51
1:B:381:PRO:HD2	1:B:482:ARG:NH2	2.25	0.51
1:C:423:ASP:O	1:C:425:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:SER:O	1:D:236:SER:C	2.54	0.51
1:B:233:ILE:O	1:B:233:ILE:CD1	2.57	0.51
1:B:402:TYR:O	1:B:406:LEU:HD12	2.10	0.51
1:A:435:ASP:N	1:A:436:PRO:HD3	2.26	0.51
1:B:283:HIS:O	2:B:601:55F:H2	2.10	0.51
1:B:331:HIS:HD2	1:B:333:ASP:H	1.59	0.51
1:C:409:TRP:CD1	1:C:471:MET:HE1	2.46	0.51
1:D:496:SER:C	1:D:498:GLN:H	2.19	0.51
1:B:487:ARG:O	1:B:491:THR:HG23	2.11	0.51
1:D:294:ARG:HD3	1:D:295:TYR:CZ	2.46	0.51
1:A:297:VAL:HG22	1:A:298:THR:H	1.76	0.50
1:A:458:TRP:O	1:A:464:LEU:HD12	2.11	0.50
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.26	0.50
1:C:211:ILE:CG2	1:C:219:VAL:HG12	2.41	0.50
1:D:425:GLN:OE1	1:D:429:TYR:CD1	2.64	0.50
1:C:184:MET:O	1:C:186:THR:N	2.40	0.50
1:C:258:ASN:C	1:C:348:CYS:HA	2.36	0.50
1:C:425:GLN:HB3	1:C:429:TYR:CD2	2.46	0.50
1:D:209:GLU:OE2	1:D:221:ARG:HD3	2.10	0.50
1:D:412:ALA:C	1:D:414:ARG:H	2.20	0.50
1:E:232:LYS:HG2	1:E:234:PHE:CE1	2.46	0.50
1:E:491:THR:HA	1:E:494:GLN:HG3	1.93	0.50
1:B:380:ALA:HB1	1:B:382:GLU:OE2	2.12	0.50
1:D:474:CYS:O	1:D:482:ARG:HD3	2.11	0.50
1:B:390:MET:HE2	1:B:396:PHE:CZ	2.47	0.50
1:C:435:ASP:O	1:C:437:SER:N	2.45	0.50
1:E:380:ALA:HA	1:E:402:TYR:CE1	2.46	0.50
1:A:199:ARG:HD2	1:A:203:ARG:NE	2.27	0.50
1:B:428:TYR:HD2	1:B:431:LEU:HD12	1.76	0.50
1:D:432:VAL:HG22	1:D:433:PRO:HD2	1.94	0.50
1:A:195:LEU:O	1:A:198:GLN:N	2.45	0.50
1:C:341:VAL:HG23	1:C:345:GLY:O	2.11	0.50
1:E:409:TRP:HA	1:E:471:MET:HE3	1.91	0.50
1:A:232:LYS:HD3	1:A:234:PHE:CZ	2.47	0.50
1:C:332:ARG:HH22	1:C:373:VAL:CB	2.24	0.50
1:E:372:ARG:O	1:E:373:VAL:HG13	2.12	0.50
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.45	0.50
1:B:409:TRP:HA	1:B:471:MET:CE	2.40	0.50
1:C:302:MET:HG3	1:C:411:ILE:CG2	2.39	0.50
1:D:240:ARG:HH11	1:D:240:ARG:CB	2.25	0.50
1:D:413:ARG:NH1	1:D:423:ASP:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:TRP:HB2	1:E:471:MET:HE3	1.92	0.50
1:D:199:ARG:HD2	1:D:203:ARG:NH2	2.26	0.49
1:D:435:ASP:N	1:D:436:PRO:HD3	2.27	0.49
1:D:457:ARG:HH11	1:D:457:ARG:HB3	1.77	0.49
1:A:372:ARG:HG3	1:A:379:MET:HE1	1.94	0.49
1:C:328:ALA:C	1:C:329:ILE:HG13	2.37	0.49
1:E:260:LEU:HD13	1:E:340:LEU:CD1	2.42	0.49
1:A:377:ARG:HH12	1:A:436:PRO:HD3	1.78	0.49
1:C:384:LEU:CD2	1:C:438:VAL:HG13	2.42	0.49
1:D:268:LYS:HB2	1:D:275:GLN:HB2	1.94	0.49
1:E:459:GLN:HE21	1:E:459:GLN:CA	2.20	0.49
1:A:489:LYS:O	1:A:493:SER:HB2	2.12	0.49
1:C:182:TYR:CD1	1:E:366:ASP:HB3	2.48	0.49
1:D:384:LEU:HB2	1:D:446:CYS:SG	2.52	0.49
1:D:459:GLN:NE2	1:D:465:ARG:NH1	2.59	0.49
1:E:498:GLN:C	1:E:499:GLU:HG2	2.36	0.49
1:C:417:ILE:HB	1:C:420:ILE:CG1	2.42	0.49
1:C:459:GLN:HE22	1:C:465:ARG:CG	2.23	0.49
1:C:486:LEU:HD13	1:C:486:LEU:C	2.37	0.49
1:E:462:GLU:O	1:E:466:VAL:HG23	2.13	0.49
1:A:198:GLN:HB3	1:A:264:ALA:HB1	1.95	0.49
1:A:309:THR:CG2	1:A:404:MET:HE2	2.32	0.49
1:B:215:ARG:CG	1:B:216:PHE:H	2.26	0.49
1:E:389:ASN:C	1:E:391:LYS:H	2.19	0.49
1:B:234:PHE:CD1	1:B:234:PHE:N	2.81	0.49
1:C:494:GLN:C	1:C:496:SER:H	2.20	0.49
1:C:197:VAL:O	1:C:198:GLN:C	2.56	0.49
1:C:377:ARG:HE	1:C:436:PRO:CD	2.26	0.49
1:E:385:ASP:OD2	1:E:387:SER:HB3	2.13	0.49
1:A:427:PRO:O	1:A:428:TYR:HB2	2.13	0.49
1:E:435:ASP:N	1:E:436:PRO:HD3	2.28	0.49
1:C:245:GLU:O	1:C:249:TYR:HD1	1.95	0.48
1:D:180:LEU:HD13	1:D:201:ILE:HD11	1.94	0.48
1:D:300:GLU:OE2	1:D:301:GLY:N	2.46	0.48
1:D:445:VAL:O	1:D:449:LYS:HA	2.12	0.48
1:E:256:HIS:CD2	1:E:256:HIS:C	2.91	0.48
1:A:455:PRO:HB2	1:A:458:TRP:CD1	2.48	0.48
1:B:208:GLN:C	1:B:209:GLU:HG3	2.38	0.48
1:B:402:TYR:O	1:B:406:LEU:CD1	2.61	0.48
1:D:261:GLY:HA3	1:D:281:ASP:OD2	2.12	0.48
1:D:391:LYS:HE2	1:D:392:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:ILE:HG12	1:E:389:ASN:N	2.28	0.48
1:A:331:HIS:HD2	1:A:333:ASP:C	2.21	0.48
1:A:432:VAL:HG23	1:A:440:GLU:HB3	1.94	0.48
1:B:381:PRO:C	1:B:383:VAL:N	2.70	0.48
1:C:261:GLY:O	1:C:280:SER:HB2	2.13	0.48
1:E:221:ARG:HH21	1:E:223:LYS:HE3	1.77	0.48
1:A:331:HIS:HE1	1:A:350:ALA:O	1.97	0.48
1:A:466:VAL:O	1:A:469:LYS:HB3	2.13	0.48
1:B:205:ILE:CG2	1:B:206:VAL:N	2.76	0.48
1:A:409:TRP:HB2	1:A:471:MET:HE3	1.94	0.48
1:D:382:GLU:OE2	1:D:482:ARG:NH2	2.36	0.48
1:D:403:ALA:O	1:D:407:VAL:HG23	2.14	0.48
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.73	0.48
1:E:377:ARG:HD3	1:E:427:PRO:O	2.13	0.48
1:B:263:ILE:HG22	1:B:264:ALA:N	2.29	0.48
1:C:402:TYR:CZ	1:C:406:LEU:HD11	2.48	0.48
1:E:381:PRO:O	1:E:384:LEU:N	2.45	0.48
1:E:409:TRP:CB	1:E:471:MET:HE3	2.44	0.48
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.62	0.48
1:D:451:ARG:O	1:D:452:PRO:C	2.55	0.48
1:A:177:LEU:HB3	1:A:227:GLU:OE2	2.14	0.48
1:C:320:ILE:CG2	1:C:321:VAL:N	2.76	0.48
1:E:248:ILE:C	1:E:250:GLN:H	2.22	0.48
1:E:366:ASP:O	1:E:367:ILE:HG23	2.14	0.48
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.53	0.48
1:A:182:TYR:CD1	1:B:366:ASP:HB3	2.49	0.48
1:B:432:VAL:HG23	1:B:433:PRO:HD2	1.95	0.48
1:C:293:ASN:ND2	1:C:424:TYR:CD2	2.82	0.48
1:B:287:SER:O	1:B:288:LEU:C	2.57	0.47
1:E:232:LYS:HE2	1:E:234:PHE:CZ	2.49	0.47
1:E:298:THR:CG2	1:E:299:VAL:N	2.77	0.47
1:B:251:THR:CG2	1:B:252:VAL:HG22	2.43	0.47
1:B:417:ILE:O	1:B:420:ILE:HG12	2.14	0.47
1:C:187:SER:O	1:C:188:GLY:C	2.57	0.47
1:C:223:LYS:HA	1:C:227:GLU:O	2.15	0.47
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.63	0.47
1:D:200:THR:O	1:D:201:ILE:C	2.57	0.47
1:A:377:ARG:O	1:A:379:MET:N	2.46	0.47
1:A:487:ARG:C	1:A:489:LYS:N	2.72	0.47
1:B:473:GLU:HB2	1:B:483:LEU:CD1	2.44	0.47
1:D:409:TRP:CZ2	1:D:413:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:O	1:A:187:SER:HB2	2.14	0.47
1:A:448:GLN:O	1:A:449:LYS:C	2.57	0.47
1:C:458:TRP:HZ3	1:C:471:MET:SD	2.37	0.47
1:D:216:PHE:CD1	1:D:232:LYS:HE2	2.49	0.47
1:E:394:GLU:O	1:E:398:ARG:HG3	2.14	0.47
1:C:248:ILE:HG22	1:C:249:TYR:N	2.27	0.47
1:C:319:GLU:CG	1:C:320:ILE:H	2.27	0.47
1:D:453:ASN:O	1:D:455:PRO:HD3	2.15	0.47
1:E:316:LEU:CD2	1:E:329:ILE:HB	2.45	0.47
1:B:389:ASN:O	1:B:391:LYS:N	2.47	0.47
1:C:308:SER:C	1:C:310:ALA:N	2.71	0.47
1:A:392:HIS:C	1:A:394:GLU:H	2.22	0.47
1:A:441:MET:O	1:A:445:VAL:HG23	2.15	0.47
1:B:205:ILE:HG22	1:B:206:VAL:N	2.29	0.47
1:C:184:MET:C	1:C:186:THR:N	2.73	0.47
1:D:417:ILE:O	1:D:420:ILE:HG12	2.14	0.47
1:D:458:TRP:O	1:D:459:GLN:CD	2.57	0.47
1:E:413:ARG:NH1	1:E:422:GLU:HB3	2.30	0.47
1:B:416:SER:HA	1:B:421:HIS:HB3	1.97	0.47
1:C:242:TRP:CE3	1:C:276:LEU:HD13	2.50	0.47
1:C:385:ASP:O	1:C:386:ASP:CB	2.63	0.47
1:D:368:ALA:CB	1:E:178:LYS:HE3	2.34	0.47
1:A:375:THR:O	1:A:379:MET:HG3	2.14	0.47
1:A:428:TYR:CE1	1:A:452:PRO:HD3	2.50	0.47
1:A:443:LYS:HE2	1:A:448:GLN:HE22	1.79	0.47
1:C:274:THR:CG2	1:C:276:LEU:HD21	2.43	0.47
1:D:397:LYS:O	1:D:400:ASP:HB2	2.14	0.47
1:E:294:ARG:HD2	1:E:295:TYR:CZ	2.50	0.47
1:D:319:GLU:HB2	1:D:328:ALA:HB2	1.98	0.47
1:D:440:GLU:O	1:D:443:LYS:HB3	2.15	0.47
1:A:412:ALA:C	1:A:414:ARG:N	2.73	0.46
1:B:420:ILE:HD12	1:B:457:ARG:HD2	1.97	0.46
1:C:248:ILE:O	1:C:251:THR:HG23	2.15	0.46
1:D:254:LEU:O	1:D:255:ARG:HB2	2.15	0.46
1:E:304:LYS:HB2	1:E:304:LYS:NZ	2.31	0.46
1:A:195:LEU:O	1:A:196:LEU:C	2.56	0.46
1:C:319:GLU:CG	1:C:320:ILE:N	2.77	0.46
1:D:392:HIS:O	1:D:393:PHE:C	2.58	0.46
1:E:417:ILE:HD11	1:E:464:LEU:CD2	2.44	0.46
1:E:478:ASN:HD22	1:E:479:GLY:N	2.12	0.46
1:A:307:LEU:HD13	1:A:307:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:VAL:HG11	1:C:441:MET:SD	2.55	0.46
1:E:469:LYS:O	1:E:473:GLU:HG3	2.15	0.46
1:A:177:LEU:HD11	1:A:263:ILE:HD13	1.97	0.46
1:C:256:HIS:O	1:C:259:ILE:N	2.45	0.46
1:D:259:ILE:O	1:D:260:LEU:C	2.57	0.46
1:D:424:TYR:CG	1:D:425:GLN:N	2.83	0.46
1:E:203:ARG:HH11	1:E:203:ARG:HG2	1.80	0.46
1:A:248:ILE:C	1:A:250:GLN:N	2.74	0.46
1:A:489:LYS:C	1:A:489:LYS:HD3	2.41	0.46
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.81	0.46
1:D:489:LYS:O	1:D:493:SER:HB2	2.16	0.46
1:A:377:ARG:C	1:A:379:MET:N	2.74	0.46
1:D:465:ARG:CZ	1:D:465:ARG:HB2	2.45	0.46
1:A:298:THR:HG22	1:A:299:VAL:N	2.29	0.46
1:A:479:GLY:HA2	1:A:482:ARG:NH1	2.31	0.46
1:B:199:ARG:CD	1:B:203:ARG:CZ	2.93	0.46
1:B:331:HIS:HE1	1:B:350:ALA:O	1.98	0.46
1:B:434:SER:O	1:B:435:ASP:HB3	2.16	0.46
1:C:237:ARG:HD3	1:C:237:ARG:C	2.40	0.46
1:C:422:GLU:OE1	1:C:422:GLU:N	2.49	0.46
1:D:362:THR:O	1:D:363:ASP:C	2.59	0.46
1:A:251:THR:O	1:A:253:MET:N	2.48	0.46
1:B:287:SER:HA	1:B:339:ILE:O	2.16	0.46
1:A:432:VAL:HG11	1:A:441:MET:SD	2.56	0.46
1:B:188:GLY:O	1:B:189:SER:CB	2.63	0.46
1:B:356:VAL:O	1:B:356:VAL:CG2	2.63	0.46
1:C:244:ARG:NH1	1:C:367:ILE:HG13	2.31	0.46
1:D:252:VAL:HB	1:D:324:GLN:HB2	1.98	0.46
1:A:473:GLU:HB3	1:A:483:LEU:CD1	2.46	0.45
1:B:216:PHE:CE2	1:B:232:LYS:HE3	2.50	0.45
1:C:232:LYS:HE2	2:C:601:55F:N13	2.31	0.45
1:C:331:HIS:CD2	1:C:331:HIS:O	2.69	0.45
1:E:302:MET:CE	1:E:467:MET:HG3	2.46	0.45
1:C:198:GLN:HB3	1:C:264:ALA:HB1	1.98	0.45
1:C:292:LEU:C	1:C:294:ARG:N	2.74	0.45
1:C:479:GLY:CA	1:C:482:ARG:HD2	2.42	0.45
1:D:293:ASN:HD22	1:D:293:ASN:HA	1.58	0.45
1:D:387:SER:O	1:D:388:ILE:C	2.59	0.45
1:E:331:HIS:CD2	1:E:331:HIS:C	2.94	0.45
1:A:180:LEU:HD13	1:A:201:ILE:HD11	1.98	0.45
1:A:476:TYR:C	1:A:478:ASN:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:MET:HG3	1:B:411:ILE:HG22	1.98	0.45
1:C:208:GLN:HG3	1:C:221:ARG:NH1	2.30	0.45
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.81	0.45
1:C:357:ARG:H	1:C:366:ASP:HB2	1.82	0.45
1:C:417:ILE:HD11	1:C:464:LEU:HD21	1.97	0.45
1:E:368:ALA:HB3	1:E:369:PRO:CD	2.42	0.45
1:B:175:THR:HA	1:C:243:PHE:CE2	2.51	0.45
1:C:229:VAL:CG2	1:C:263:ILE:HD12	2.47	0.45
1:C:454:ILE:HD11	1:C:475:TRP:HZ3	1.78	0.45
1:D:381:PRO:HG3	1:D:445:VAL:CG1	2.47	0.45
1:A:413:ARG:NH2	1:A:425:GLN:HG3	2.31	0.45
1:A:417:ILE:HG13	1:A:420:ILE:HG13	1.98	0.45
1:C:215:ARG:HE	1:C:215:ARG:H	1.62	0.45
1:C:287:SER:HA	1:C:339:ILE:O	2.16	0.45
1:C:494:GLN:HG3	1:C:497:GLN:CD	2.42	0.45
1:A:331:HIS:CD2	1:A:333:ASP:C	2.95	0.45
1:D:211:ILE:O	1:D:211:ILE:CG2	2.62	0.45
1:A:248:ILE:C	1:A:250:GLN:H	2.25	0.45
1:A:254:LEU:HD11	1:A:259:ILE:HG21	1.99	0.45
1:C:298:THR:HG22	1:C:300:GLU:N	2.11	0.45
1:D:240:ARG:NH1	1:D:240:ARG:HB2	2.32	0.45
1:D:367:ILE:HG13	1:D:368:ALA:N	2.31	0.45
1:E:308:SER:O	1:E:309:THR:C	2.60	0.45
1:C:215:ARG:N	1:C:215:ARG:NE	2.62	0.45
1:C:307:LEU:HD23	1:C:307:LEU:C	2.41	0.45
1:E:442:ARG:O	1:E:446:CYS:HB2	2.17	0.45
1:A:199:ARG:HD2	1:A:203:ARG:NH2	2.31	0.45
1:B:256:HIS:CD2	1:B:258:ASN:H	2.34	0.45
1:C:195:LEU:O	1:C:196:LEU:C	2.58	0.45
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.46	0.44
1:A:404:MET:O	1:A:404:MET:HG2	2.17	0.44
1:B:443:LYS:HE2	1:B:448:GLN:NE2	2.33	0.44
1:C:270:ASN:O	1:C:271:GLY:C	2.59	0.44
1:C:402:TYR:CD1	1:C:402:TYR:C	2.95	0.44
1:C:434:SER:O	1:C:435:ASP:C	2.60	0.44
1:D:313:LEU:HD13	1:D:334:LEU:HD11	1.98	0.44
1:E:293:ASN:ND2	1:E:424:TYR:CD2	2.85	0.44
1:E:316:LEU:HD23	1:E:329:ILE:HB	2.00	0.44
1:A:239:GLU:O	1:A:242:TRP:HB3	2.17	0.44
1:A:471:MET:O	1:A:475:TRP:CG	2.70	0.44
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:HA	1:C:238:GLU:HG3	1.99	0.44
1:C:287:SER:O	1:C:288:LEU:C	2.59	0.44
1:C:341:VAL:HG13	1:C:341:VAL:O	2.17	0.44
1:C:375:THR:O	1:C:376:LYS:C	2.60	0.44
1:D:258:ASN:O	1:D:348:CYS:HA	2.17	0.44
1:D:462:GLU:O	1:D:463:ALA:C	2.59	0.44
1:A:257:GLU:HG2	1:A:257:GLU:O	2.15	0.44
1:B:259:ILE:O	1:B:260:LEU:C	2.60	0.44
1:C:178:LYS:NZ	1:E:367:ILE:CD1	2.81	0.44
1:C:333:ASP:O	1:C:333:ASP:CG	2.60	0.44
1:C:337:LYS:C	1:C:339:ILE:H	2.25	0.44
1:C:393:PHE:O	1:C:396:PHE:HB2	2.18	0.44
1:D:291:TYR:HB2	1:D:341:VAL:HG11	1.98	0.44
1:D:376:LYS:CA	1:D:379:MET:HE3	2.48	0.44
1:E:184:MET:HE3	1:E:184:MET:HB3	1.88	0.44
1:E:298:THR:HG22	1:E:299:VAL:H	1.81	0.44
1:A:195:LEU:O	1:A:197:VAL:N	2.51	0.44
1:A:381:PRO:HG3	1:A:445:VAL:CG1	2.48	0.44
1:B:270:ASN:O	1:B:271:GLY:C	2.59	0.44
1:B:331:HIS:CD2	1:B:333:ASP:H	2.36	0.44
1:C:302:MET:HE3	1:C:467:MET:HG3	1.99	0.44
1:C:377:ARG:HG3	1:C:436:PRO:HG2	1.99	0.44
1:E:334:LEU:O	1:E:335:LYS:CB	2.65	0.44
1:A:350:ALA:O	1:A:351:ASP:CB	2.66	0.44
1:B:313:LEU:HD22	1:B:334:LEU:HD11	2.00	0.44
1:C:332:ARG:HH22	1:C:373:VAL:HG21	1.82	0.44
1:D:374:GLY:O	1:D:379:MET:HE2	2.18	0.44
1:E:302:MET:HG2	1:E:467:MET:HE2	2.00	0.44
1:A:194:PRO:HB2	1:A:197:VAL:HG23	1.98	0.44
1:B:431:LEU:HD13	1:B:444:VAL:CG1	2.48	0.44
1:B:456:ASN:O	1:B:457:ARG:C	2.61	0.44
1:C:312:GLY:C	1:C:314:ALA:N	2.75	0.44
1:C:457:ARG:HD2	1:C:457:ARG:C	2.43	0.44
1:D:310:ALA:CA	1:D:404:MET:HE1	2.40	0.44
1:D:448:GLN:O	1:D:449:LYS:C	2.61	0.44
1:E:367:ILE:HD12	1:E:367:ILE:H	1.82	0.44
1:A:182:TYR:O	1:A:183:ASP:C	2.61	0.44
1:A:470:ILE:CA	1:A:473:GLU:HB2	2.43	0.44
1:E:334:LEU:HD23	1:E:334:LEU:HA	1.73	0.44
1:B:181:ILE:O	1:B:184:MET:HG2	2.18	0.44
1:B:382:GLU:CD	1:B:482:ARG:HH12	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:SER:HA	1:B:420:ILE:O	2.18	0.44
1:B:424:TYR:CD2	1:B:424:TYR:C	2.95	0.44
1:C:434:SER:C	1:C:436:PRO:CD	2.91	0.44
1:C:464:LEU:H	1:C:464:LEU:CD2	2.31	0.44
1:E:194:PRO:O	1:E:195:LEU:C	2.61	0.44
1:B:331:HIS:CD2	1:B:331:HIS:C	2.95	0.43
1:C:259:ILE:O	1:C:260:LEU:C	2.61	0.43
1:C:331:HIS:CD2	1:C:334:LEU:N	2.86	0.43
1:C:332:ARG:HH22	1:C:373:VAL:HG11	1.83	0.43
1:C:378:TYR:CD1	1:C:378:TYR:N	2.86	0.43
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.13	0.43
1:A:248:ILE:HD13	1:A:355:ALA:HB3	2.00	0.43
1:A:372:ARG:CG	1:A:379:MET:HE1	2.48	0.43
1:A:394:GLU:O	1:A:398:ARG:HG2	2.19	0.43
1:B:234:PHE:CE1	1:B:278:LEU:HD22	2.53	0.43
1:C:215:ARG:H	1:C:215:ARG:NE	2.16	0.43
1:C:487:ARG:HH22	1:C:490:LYS:HD2	1.82	0.43
1:A:254:LEU:C	1:A:254:LEU:HD12	2.43	0.43
1:A:375:THR:O	1:A:377:ARG:N	2.51	0.43
1:A:393:PHE:CG	1:A:393:PHE:O	2.71	0.43
1:C:294:ARG:HD3	1:C:295:TYR:CZ	2.53	0.43
1:D:178:LYS:H	1:D:178:LYS:CD	2.31	0.43
1:E:242:TRP:CD1	1:E:276:LEU:HB3	2.54	0.43
1:A:270:ASN:O	1:A:271:GLY:C	2.62	0.43
1:A:326:LYS:HG3	1:A:326:LYS:O	2.18	0.43
1:A:428:TYR:N	1:A:428:TYR:CD1	2.86	0.43
1:B:447:GLU:C	1:B:449:LYS:H	2.26	0.43
1:D:469:LYS:HE2	1:D:473:GLU:CD	2.42	0.43
1:E:319:GLU:OE2	1:E:360:SER:HB3	2.18	0.43
1:E:478:ASN:ND2	1:E:479:GLY:N	2.66	0.43
1:A:431:LEU:HB3	1:A:444:VAL:HG11	2.00	0.43
1:A:473:GLU:HB3	1:A:483:LEU:CG	2.49	0.43
1:B:457:ARG:C	1:B:459:GLN:H	2.27	0.43
1:C:224:TRP:O	1:C:225:ARG:HB2	2.18	0.43
1:C:416:SER:HA	1:C:421:HIS:HB3	2.01	0.43
1:E:409:TRP:CH2	1:E:413:ARG:HD2	2.53	0.43
1:A:232:LYS:HE3	2:A:601:55F:N13	2.34	0.43
1:A:470:ILE:HD13	1:A:488:ILE:HG23	1.99	0.43
1:C:187:SER:O	1:C:189:SER:N	2.52	0.43
1:C:428:TYR:HE2	1:C:452:PRO:CD	2.30	0.43
1:C:468:ALA:HA	1:C:471:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:PHE:CD1	1:D:234:PHE:N	2.85	0.43
1:D:479:GLY:HA2	1:D:482:ARG:CZ	2.49	0.43
1:E:178:LYS:HB2	1:E:178:LYS:HE2	1.66	0.43
1:E:200:THR:O	1:E:201:ILE:C	2.62	0.43
1:A:184:MET:O	1:A:185:THR:C	2.62	0.43
1:A:224:TRP:CZ3	1:A:225:ARG:HD2	2.54	0.43
1:A:366:ASP:O	1:A:367:ILE:C	2.61	0.43
1:A:454:ILE:O	1:A:455:PRO:C	2.62	0.43
1:C:362:THR:O	1:C:362:THR:HG22	2.18	0.43
1:C:398:ARG:O	1:C:399:ALA:C	2.62	0.43
1:A:431:LEU:HD13	1:A:444:VAL:CG1	2.48	0.43
1:C:186:THR:O	1:C:186:THR:HG23	2.18	0.43
1:D:214:GLY:HA3	1:D:216:PHE:CE2	2.54	0.43
1:D:380:ALA:HB1	1:D:382:GLU:OE2	2.19	0.43
1:E:179:ASP:O	1:E:180:LEU:C	2.61	0.43
1:E:376:LYS:HA	1:E:379:MET:SD	2.59	0.43
1:A:224:TRP:CZ2	1:A:225:ARG:HD2	2.54	0.43
1:B:442:ARG:O	1:B:446:CYS:HB2	2.19	0.43
1:C:335:LYS:HG2	1:C:336:SER:H	1.76	0.43
1:C:425:GLN:HB3	1:C:429:TYR:CG	2.54	0.43
1:C:485:ALA:C	1:C:487:ARG:N	2.76	0.43
1:E:252:VAL:HG23	1:E:253:MET:H	1.83	0.43
1:B:381:PRO:HG3	1:B:445:VAL:CG1	2.48	0.43
1:B:436:PRO:HB3	1:B:441:MET:HG2	2.01	0.43
1:C:270:ASN:O	1:C:274:THR:N	2.52	0.43
1:C:299:VAL:HG21	1:C:417:ILE:HG12	2.00	0.43
1:C:389:ASN:HD22	1:C:390:MET:N	2.16	0.43
1:E:450:LEU:O	1:E:451:ARG:HD3	2.19	0.43
1:B:258:ASN:O	1:B:348:CYS:HA	2.18	0.42
1:C:380:ALA:HA	1:C:402:TYR:CE1	2.55	0.42
1:D:431:LEU:HD22	1:D:444:VAL:CG1	2.47	0.42
1:D:458:TRP:CG	1:D:464:LEU:HD12	2.53	0.42
1:E:263:ILE:HG22	1:E:264:ALA:N	2.34	0.42
1:C:398:ARG:HB3	1:C:482:ARG:NH1	2.30	0.42
1:E:215:ARG:H	1:E:215:ARG:HG2	1.54	0.42
1:E:305:LEU:HD22	1:E:347:CYS:SG	2.58	0.42
1:A:373:VAL:HG23	1:A:374:GLY:N	2.34	0.42
1:A:495:LEU:O	1:A:495:LEU:HD12	2.19	0.42
1:C:308:SER:O	1:C:310:ALA:N	2.53	0.42
1:C:428:TYR:HE2	1:C:452:PRO:HD3	1.84	0.42
1:D:428:TYR:O	1:D:429:TYR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ILE:C	1:E:250:GLN:N	2.77	0.42
1:A:235:SER:O	1:A:236:SER:C	2.62	0.42
1:B:182:TYR:C	1:B:182:TYR:CD2	2.97	0.42
1:B:292:LEU:O	1:B:414:ARG:HD3	2.19	0.42
1:C:177:LEU:O	1:C:178:LYS:C	2.63	0.42
1:E:319:GLU:CD	1:E:360:SER:HB3	2.44	0.42
1:E:382:GLU:H	1:E:382:GLU:HG3	1.45	0.42
1:A:252:VAL:HG23	1:A:253:MET:H	1.82	0.42
1:A:394:GLU:C	1:A:396:PHE:N	2.76	0.42
1:A:432:VAL:CG2	1:A:440:GLU:HB3	2.50	0.42
1:A:486:LEU:O	1:A:486:LEU:HD23	2.20	0.42
1:C:175:THR:HG22	1:C:176:THR:N	2.34	0.42
1:C:237:ARG:HD3	1:C:237:ARG:O	2.19	0.42
1:C:298:THR:O	1:C:301:GLY:N	2.50	0.42
1:C:326:LYS:HB2	1:C:327:PRO:HD2	2.01	0.42
1:D:479:GLY:HA2	1:D:482:ARG:NE	2.34	0.42
1:E:235:SER:O	1:E:238:GLU:N	2.50	0.42
1:E:302:MET:HG3	1:E:411:ILE:HG22	2.01	0.42
1:A:283:HIS:O	1:A:284:GLU:C	2.61	0.42
1:B:181:ILE:O	1:B:182:TYR:C	2.61	0.42
1:E:252:VAL:HG23	1:E:253:MET:N	2.34	0.42
1:A:177:LEU:H	1:A:227:GLU:CD	2.27	0.42
1:B:254:LEU:HD11	1:B:259:ILE:HD13	2.01	0.42
1:C:312:GLY:O	1:C:315:HIS:N	2.53	0.42
1:C:332:ARG:O	1:C:333:ASP:HB2	2.19	0.42
1:D:306:ALA:HB1	1:D:492:LEU:HD21	2.01	0.42
1:D:432:VAL:O	1:D:433:PRO:O	2.37	0.42
1:E:302:MET:HE3	1:E:467:MET:HG3	2.01	0.42
1:E:367:ILE:HB	1:E:370:ASN:ND2	2.35	0.42
1:E:462:GLU:HG2	1:E:498:GLN:HE22	1.84	0.42
1:A:215:ARG:C	1:A:217:GLY:N	2.75	0.42
1:A:377:ARG:NH1	1:A:436:PRO:HD3	2.34	0.42
1:A:420:ILE:HD12	1:A:457:ARG:NH1	2.35	0.42
1:A:427:PRO:C	1:A:428:TYR:HD1	2.28	0.42
1:A:443:LYS:HE2	1:A:448:GLN:HE21	1.81	0.42
1:B:178:LYS:HG2	1:C:368:ALA:CB	2.49	0.42
1:B:417:ILE:HD11	1:B:464:LEU:HD22	2.01	0.42
1:B:455:PRO:HD2	1:B:458:TRP:CE2	2.53	0.42
1:D:364:THR:C	1:D:365:ILE:HD12	2.45	0.42
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.87	0.42
1:B:464:LEU:HA	1:B:464:LEU:HD12	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLU:HG3	1:C:249:TYR:CE1	2.54	0.42
1:C:311:SER:HA	1:C:489:LYS:HG3	2.01	0.42
1:D:443:LYS:HG3	1:D:448:GLN:NE2	2.34	0.42
1:E:292:LEU:HA	1:E:292:LEU:HD12	1.66	0.42
1:E:311:SER:HA	1:E:489:LYS:HD2	2.01	0.42
1:A:422:GLU:OE1	1:A:455:PRO:HG2	2.19	0.42
1:A:479:GLY:HA2	1:A:482:ARG:HH12	1.85	0.42
1:B:215:ARG:HH11	1:B:215:ARG:HG2	1.85	0.42
1:B:385:ASP:HB2	1:B:442:ARG:HH21	1.85	0.42
1:B:409:TRP:CB	1:B:471:MET:HE3	2.50	0.42
1:C:473:GLU:HG2	1:C:476:TYR:OH	2.20	0.42
1:D:293:ASN:ND2	1:D:424:TYR:CB	2.83	0.42
1:D:498:GLN:C	1:D:499:GLU:HG3	2.45	0.42
1:E:270:ASN:O	1:E:271:GLY:C	2.62	0.42
1:E:343:LYS:C	1:E:345:GLY:H	2.28	0.42
1:E:423:ASP:OD2	1:E:423:ASP:N	2.42	0.42
1:A:252:VAL:HB	1:A:324:GLN:HB3	2.02	0.41
1:B:444:VAL:HG13	1:B:450:LEU:HD12	2.01	0.41
1:C:256:HIS:O	1:C:257:GLU:C	2.62	0.41
1:D:358:HIS:HB2	1:D:393:PHE:CD1	2.55	0.41
1:E:235:SER:O	1:E:236:SER:C	2.62	0.41
1:E:288:LEU:HG	1:E:292:LEU:HD22	2.01	0.41
1:A:494:GLN:C	1:A:496:SER:H	2.28	0.41
1:C:289:PHE:CD2	1:C:337:LYS:HE2	2.56	0.41
1:C:420:ILE:O	1:C:420:ILE:CG1	2.67	0.41
1:C:459:GLN:HA	1:C:459:GLN:NE2	2.35	0.41
1:D:173:GLU:H	1:D:173:GLU:CD	2.27	0.41
1:D:389:ASN:ND2	1:D:389:ASN:C	2.79	0.41
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.55	0.41
1:A:213:LYS:HE2	1:A:213:LYS:HB3	1.73	0.41
1:A:332:ARG:HH22	1:A:373:VAL:HG11	1.83	0.41
1:A:401:ILE:HD11	1:A:485:ALA:HB2	2.01	0.41
1:A:464:LEU:HD13	1:A:464:LEU:O	2.20	0.41
1:B:177:LEU:H	1:B:227:GLU:CD	2.28	0.41
1:C:234:PHE:CD1	1:C:234:PHE:N	2.88	0.41
1:C:457:ARG:C	1:C:459:GLN:H	2.29	0.41
1:D:376:LYS:HG3	1:D:379:MET:HE3	2.02	0.41
1:E:285:HIS:HB3	1:E:341:VAL:HG22	2.01	0.41
1:A:335:LYS:HE3	1:A:337:LYS:HB2	2.02	0.41
1:B:435:ASP:N	1:B:436:PRO:HD3	2.35	0.41
1:B:451:ARG:NH2	1:B:475:TRP:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:HIS:C	1:C:258:ASN:N	2.79	0.41
1:D:244:ARG:HH22	1:D:366:ASP:CG	2.28	0.41
1:A:382:GLU:OE2	1:A:482:ARG:NH2	2.44	0.41
1:A:470:ILE:HG13	1:A:470:ILE:H	1.67	0.41
1:C:232:LYS:HD2	1:C:234:PHE:CE1	2.55	0.41
1:A:259:ILE:CD1	1:A:316:LEU:HG	2.50	0.41
1:A:343:LYS:HG2	3:A:9:PO4:P	2.60	0.41
1:C:289:PHE:HB3	1:C:337:LYS:HG2	2.03	0.41
1:C:327:PRO:O	1:C:329:ILE:HG13	2.20	0.41
1:C:372:ARG:CZ	1:C:438:VAL:HG21	2.50	0.41
1:C:384:LEU:O	1:C:442:ARG:HD2	2.21	0.41
1:D:336:SER:HB3	1:D:410:GLU:OE1	2.20	0.41
1:E:381:PRO:O	1:E:382:GLU:C	2.62	0.41
1:A:234:PHE:HE1	1:A:278:LEU:HD22	1.85	0.41
1:A:315:HIS:O	1:A:315:HIS:ND1	2.53	0.41
1:A:409:TRP:CE2	1:A:452:PRO:HB3	2.56	0.41
1:A:487:ARG:HD2	1:A:487:ARG:HA	1.83	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.84	0.41
1:C:265:ALA:CB	1:C:278:LEU:HD12	2.51	0.41
1:C:354:LEU:HD23	1:C:354:LEU:HA	1.86	0.41
1:D:306:ALA:CB	1:D:492:LEU:HD21	2.51	0.41
1:D:308:SER:OG	1:D:309:THR:N	2.53	0.41
1:E:377:ARG:NH1	3:E:2:PO4:O1	2.40	0.41
1:E:382:GLU:OE2	1:E:482:ARG:NH1	2.49	0.41
1:A:263:ILE:HB	1:A:279:VAL:O	2.20	0.41
1:A:367:ILE:HD12	1:A:370:ASN:CB	2.49	0.41
1:C:178:LYS:HZ2	1:E:367:ILE:CD1	2.34	0.41
1:C:303:ILE:HG21	1:C:496:SER:CB	2.51	0.41
1:C:336:SER:O	1:C:339:ILE:HB	2.21	0.41
1:C:398:ARG:O	1:C:400:ASP:N	2.54	0.41
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.85	0.41
1:D:293:ASN:ND2	1:D:424:TYR:HB3	2.36	0.41
1:D:376:LYS:HG3	1:D:379:MET:CE	2.50	0.41
1:A:237:ARG:HB3	1:A:237:ARG:HH11	1.85	0.41
1:A:350:ALA:O	1:A:351:ASP:HB3	2.21	0.41
1:A:375:THR:C	1:A:377:ARG:H	2.29	0.41
1:A:382:GLU:H	1:A:382:GLU:CD	2.29	0.41
1:C:331:HIS:CD2	1:C:333:ASP:C	2.99	0.41
1:C:451:ARG:CG	1:C:475:TRP:HB3	2.49	0.41
1:C:463:ALA:O	1:C:464:LEU:C	2.64	0.41
1:D:376:LYS:HA	1:D:379:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:HB3	1:A:483:LEU:HD11	2.03	0.41
1:B:252:VAL:CG2	1:B:326:LYS:HA	2.43	0.41
1:B:258:ASN:C	1:B:348:CYS:HA	2.46	0.41
1:B:307:LEU:O	1:B:307:LEU:HD22	2.20	0.41
1:B:385:ASP:O	1:B:387:SER:N	2.54	0.41
1:B:447:GLU:C	1:B:449:LYS:N	2.80	0.41
1:C:452:PRO:HB2	1:C:475:TRP:CH2	2.56	0.41
1:D:414:ARG:HD2	1:D:424:TYR:HB2	2.03	0.41
1:E:356:VAL:CG2	1:E:393:PHE:HE1	2.30	0.41
1:A:308:SER:O	1:A:309:THR:C	2.64	0.40
1:A:317:HIS:ND1	1:A:397:LYS:HG2	2.36	0.40
1:A:342:LYS:HB3	3:A:9:PO4:O3	2.21	0.40
1:B:216:PHE:O	1:B:238:GLU:HG3	2.21	0.40
1:B:251:THR:O	1:B:252:VAL:C	2.64	0.40
1:C:302:MET:CE	1:C:467:MET:HG3	2.50	0.40
1:D:343:LYS:HB2	3:D:13:PO4:P	2.61	0.40
1:E:443:LYS:HE2	1:E:448:GLN:HE21	1.87	0.40
1:A:181:ILE:O	1:A:185:THR:HG23	2.20	0.40
1:B:233:ILE:O	1:B:233:ILE:CG1	2.68	0.40
1:C:416:SER:C	1:C:417:ILE:HG13	2.47	0.40
1:C:476:TYR:O	1:C:477:ALA:C	2.63	0.40
1:D:178:LYS:N	1:D:178:LYS:CD	2.83	0.40
1:B:194:PRO:O	1:B:197:VAL:N	2.54	0.40
1:B:300:GLU:HG3	1:B:501:ILE:HD13	2.03	0.40
1:B:337:LYS:HD2	3:B:23:PO4:O2	2.20	0.40
1:B:365:ILE:HG13	1:B:365:ILE:O	2.22	0.40
1:C:182:TYR:CE2	1:C:186:THR:HG21	2.56	0.40
1:C:324:GLN:O	1:C:325:GLY:C	2.64	0.40
1:C:428:TYR:CD2	1:C:428:TYR:N	2.88	0.40
1:C:487:ARG:C	1:C:489:LYS:N	2.79	0.40
1:D:243:PHE:CD2	1:E:175:THR:HA	2.56	0.40
1:D:303:ILE:O	1:D:304:LYS:C	2.64	0.40
1:E:432:VAL:HG22	1:E:433:PRO:CD	2.52	0.40
1:E:497:GLN:O	1:E:499:GLU:N	2.54	0.40
1:A:205:ILE:HG22	1:A:206:VAL:N	2.36	0.40
1:B:372:ARG:NH2	1:B:438:VAL:HG11	2.36	0.40
1:B:431:LEU:HD22	1:B:450:LEU:HD13	2.04	0.40
1:C:354:LEU:HD22	1:C:373:VAL:CG1	2.52	0.40
1:C:476:TYR:C	1:C:478:ASN:N	2.74	0.40
1:D:331:HIS:CD2	1:D:331:HIS:C	2.99	0.40
1:A:181:ILE:O	1:A:184:MET:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LYS:O	1:A:447:GLU:HB2	2.21	0.40
1:B:487:ARG:HE	1:B:491:THR:HG22	1.86	0.40
1:C:256:HIS:O	1:C:258:ASN:N	2.54	0.40
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.89	0.40
1:D:412:ALA:O	1:D:414:ARG:N	2.55	0.40
1:E:294:ARG:HD2	1:E:295:TYR:CE1	2.57	0.40
1:E:302:MET:CG	1:E:467:MET:HE2	2.52	0.40
1:E:333:ASP:HB2	1:E:354:LEU:HD12	2.04	0.40
1:E:473:GLU:OE1	1:E:483:LEU:HD21	2.21	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	324/342 (95%)	240 (74%)	61 (19%)	23 (7%)	1	5
1	B	318/342 (93%)	259 (81%)	43 (14%)	16 (5%)	1	10
1	C	328/342 (96%)	239 (73%)	61 (19%)	28 (8%)	0	4
1	D	328/342 (96%)	266 (81%)	51 (16%)	11 (3%)	3	16
1	E	328/342 (96%)	272 (83%)	37 (11%)	19 (6%)	1	8
All	All	1626/1710 (95%)	1276 (78%)	253 (16%)	97 (6%)	1	7

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	VAL
1	A	447	GLU
1	B	191	SER
1	B	252	VAL
1	B	386	ASP

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Mol	Chain	Res	Type
1	C	191	SER
1	C	211	ILE
1	C	252	VAL
1	C	255	ARG
1	C	271	GLY
1	C	333	ASP
1	C	342	LYS
1	C	346	THR
1	C	376	LYS
1	C	432	VAL
1	C	433	PRO
1	D	252	VAL
1	D	255	ARG
1	D	269	ASP
1	D	388	ILE
1	D	433	PRO
1	E	252	VAL
1	E	433	PRO
1	A	271	GLY
1	A	318	MET
1	A	333	ASP
1	A	376	LYS
1	A	378	TYR
1	A	393	PHE
1	A	479	GLY
1	B	188	GLY
1	B	192	GLY
1	B	382	GLU
1	C	188	GLY
1	C	386	ASP
1	C	436	PRO
1	C	458	TRP
1	E	271	GLY
1	E	322	GLY
1	E	335	LYS
1	E	351	ASP
1	A	260	LEU
1	A	386	ASP
1	A	387	SER
1	A	448	GLN
1	B	190	GLY
1	B	335	LYS

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Mol	Chain	Res	Type
1	B	366	ASP
1	C	185	THR
1	C	186	THR
1	C	210	SER
1	C	218	GLU
1	C	366	ASP
1	C	399	ALA
1	C	484	THR
1	D	413	ARG
1	D	499	GLU
1	E	188	GLY
1	E	333	ASP
1	E	371	HIS
1	A	196	LEU
1	A	289	PHE
1	A	477	ALA
1	B	189	SER
1	B	269	ASP
1	B	271	GLY
1	B	333	ASP
1	B	390	MET
1	C	257	GLU
1	C	345	GLY
1	C	455	PRO
1	D	355	ALA
1	D	386	ASP
1	E	260	LEU
1	E	336	SER
1	E	460	SER
1	E	498	GLN
1	A	188	GLY
1	A	272	THR
1	A	457	ARG
1	B	436	PRO
1	B	448	GLN
1	C	363	ASP
1	C	427	PRO
1	E	344	ASN
1	E	355	ALA
1	E	369	PRO
1	E	381	PRO
1	E	455	PRO

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	255	ARG
1	D	186	THR
1	C	327	PRO
1	E	211	ILE
1	A	454	ILE
1	D	367	ILE
1	A	455	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	281/294 (96%)	259 (92%)	22 (8%)	11	37
1	B	278/294 (95%)	252 (91%)	26 (9%)	8	29
1	C	282/294 (96%)	261 (93%)	21 (7%)	13	38
1	D	282/294 (96%)	256 (91%)	26 (9%)	8	30
1	E	282/294 (96%)	254 (90%)	28 (10%)	7	27
All	All	1405/1470 (96%)	1282 (91%)	123 (9%)	9	31

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	MET
1	A	196	LEU
1	A	199	ARG
1	A	209	GLU
1	A	229	VAL
1	A	237	ARG
1	A	254	LEU
1	A	267	ASN
1	A	269	ASP
1	A	278	LEU
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	292	LEU
1	A	294	ARG
1	A	296	THR
1	A	307	LEU
1	A	334	LEU
1	A	341	VAL
1	A	378	TYR
1	A	428	TYR
1	A	430	ASP
1	A	464	LEU
1	A	484	THR
1	B	207	LEU
1	B	209	GLU
1	B	229	VAL
1	B	233	ILE
1	B	234	PHE
1	B	268	LYS
1	B	269	ASP
1	B	278	LEU
1	B	292	LEU
1	B	294	ARG
1	B	307	LEU
1	B	316	LEU
1	B	341	VAL
1	B	351	ASP
1	B	356	VAL
1	B	362	THR
1	B	382	GLU
1	B	390	MET
1	B	406	LEU
1	B	449	LYS
1	B	451	ARG
1	B	464	LEU
1	B	465	ARG
1	B	486	LEU
1	B	491	THR
1	B	492	LEU
1	C	178	LYS
1	C	186	THR
1	C	209	GLU
1	C	215	ARG
1	C	241	SER

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Mol	Chain	Res	Type
1	C	247	GLU
1	C	257	GLU
1	C	259	ILE
1	C	267	ASN
1	C	268	LYS
1	C	298	THR
1	C	332	ARG
1	C	334	LEU
1	C	352	LEU
1	C	364	THR
1	C	367	ILE
1	C	402	TYR
1	C	415	CYS
1	C	427	PRO
1	C	430	ASP
1	C	483	LEU
1	D	191	SER
1	D	195	LEU
1	D	209	GLU
1	D	211	ILE
1	D	231	VAL
1	D	244	ARG
1	D	247	GLU
1	D	248	ILE
1	D	267	ASN
1	D	269	ASP
1	D	278	LEU
1	D	284	GLU
1	D	292	LEU
1	D	296	THR
1	D	300	GLU
1	D	321	VAL
1	D	371	HIS
1	D	376	LYS
1	D	377	ARG
1	D	381	PRO
1	D	382	GLU
1	D	429	TYR
1	D	431	LEU
1	D	457	ARG
1	D	486	LEU
1	D	491	THR

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Mol	Chain	Res	Type
1	E	184	MET
1	E	204	THR
1	E	209	GLU
1	E	215	ARG
1	E	253	MET
1	E	267	ASN
1	E	278	LEU
1	E	292	LEU
1	E	294	ARG
1	E	297	VAL
1	E	304	LYS
1	E	307	LEU
1	E	316	LEU
1	E	341	VAL
1	E	342	LYS
1	E	366	ASP
1	E	367	ILE
1	E	376	LYS
1	E	379	MET
1	E	382	GLU
1	E	388	ILE
1	E	423	ASP
1	E	455	PRO
1	E	464	LEU
1	E	486	LEU
1	E	491	THR
1	E	492	LEU
1	E	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	256	HIS
1	A	267	ASN
1	A	285	HIS
1	A	331	HIS
1	A	392	HIS
1	A	425	GLN
1	A	448	GLN
1	B	250	GLN
1	B	256	HIS

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Mol	Chain	Res	Type
1	B	258	ASN
1	B	315	HIS
1	B	331	HIS
1	B	389	ASN
1	B	392	HIS
1	B	425	GLN
1	B	448	GLN
1	B	459	GLN
1	C	250	GLN
1	C	256	HIS
1	C	258	ASN
1	C	267	ASN
1	C	285	HIS
1	C	324	GLN
1	C	331	HIS
1	C	370	ASN
1	C	389	ASN
1	C	392	HIS
1	C	425	GLN
1	C	453	ASN
1	C	459	GLN
1	C	478	ASN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	270	ASN
1	D	275	GLN
1	D	293	ASN
1	D	324	GLN
1	D	331	HIS
1	D	358	HIS
1	D	370	ASN
1	D	389	ASN
1	D	448	GLN
1	D	459	GLN
1	D	497	GLN
1	D	498	GLN
1	E	208	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	315	HIS

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Mol	Chain	Res	Type
1	E	370	ASN
1	E	389	ASN
1	E	425	GLN
1	E	448	GLN
1	E	459	GLN
1	E	478	ASN
1	E	498	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	55F	C	601	-	30,30,30	1.59	8 (26%)	40,43,43	1.38	7 (17%)
3	PO4	A	9	-	4,4,4	1.67	1 (25%)	6,6,6	0.48	0
3	PO4	A	21	-	4,4,4	1.75	1 (25%)	6,6,6	0.49	0
3	PO4	B	23	-	4,4,4	1.79	2 (50%)	6,6,6	0.47	0
3	PO4	E	2	-	4,4,4	1.75	2 (50%)	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	55F	D	601	-	30,30,30	1.58	8 (26%)	40,43,43	1.40	9 (22%)
3	PO4	B	12	-	4,4,4	1.81	2 (50%)	6,6,6	0.44	0
3	PO4	D	24	-	4,4,4	1.74	1 (25%)	6,6,6	0.46	0
3	PO4	E	1	-	4,4,4	1.74	1 (25%)	6,6,6	0.49	0
2	55F	A	601	-	30,30,30	1.55	8 (26%)	40,43,43	1.40	7 (17%)
3	PO4	D	13	-	4,4,4	1.69	0	6,6,6	0.50	0
3	PO4	D	14	-	4,4,4	1.82	1 (25%)	6,6,6	0.46	0
2	55F	B	601	-	30,30,30	1.57	8 (26%)	40,43,43	1.47	6 (15%)
3	PO4	E	22	-	4,4,4	1.71	0	6,6,6	0.49	0
2	55F	E	601	-	30,30,30	1.40	7 (23%)	40,43,43	1.37	7 (17%)
3	PO4	C	10	-	4,4,4	1.63	0	6,6,6	0.48	0
3	PO4	A	26	-	4,4,4	1.71	1 (25%)	6,6,6	0.47	0
3	PO4	B	6	-	4,4,4	1.71	1 (25%)	6,6,6	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	55F	C	601	-	-	6/12/12/12	0/4/4/4
2	55F	D	601	-	-	6/12/12/12	0/4/4/4
2	55F	A	601	-	-	6/12/12/12	0/4/4/4
2	55F	B	601	-	-	4/12/12/12	0/4/4/4
2	55F	E	601	-	-	4/12/12/12	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	55F	C20-N21	3.19	1.38	1.34
2	C	601	55F	C16-N21	3.19	1.39	1.34
2	B	601	55F	C20-N21	3.11	1.38	1.34
2	D	601	55F	C20-N21	3.01	1.38	1.34
2	C	601	55F	C2-N3	3.00	1.38	1.32
2	B	601	55F	C16-N21	2.91	1.38	1.34
2	B	601	55F	C2-N3	2.90	1.38	1.32
2	D	601	55F	C16-N21	2.88	1.38	1.34
2	D	601	55F	C1-N6	2.85	1.38	1.32
2	A	601	55F	C10-C9	2.85	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	55F	C10-C9	2.85	1.42	1.37
2	C	601	55F	C7-C8	2.83	1.42	1.36
2	A	601	55F	C8-C9	2.77	1.43	1.39
2	B	601	55F	C7-C8	2.76	1.42	1.36
2	A	601	55F	C1-N6	2.76	1.37	1.32
2	D	601	55F	C10-C9	2.75	1.42	1.37
2	D	601	55F	C14-N13	-2.72	1.28	1.33
2	B	601	55F	C1-N6	2.67	1.37	1.32
2	A	601	55F	C7-C8	2.66	1.42	1.36
2	C	601	55F	C20-N21	2.63	1.38	1.34
2	C	601	55F	C1-N6	2.59	1.37	1.32
2	C	601	55F	C8-C9	2.59	1.43	1.39
2	B	601	55F	C10-C9	2.58	1.42	1.37
2	A	601	55F	C2-N3	2.58	1.37	1.32
2	D	601	55F	C7-C8	2.54	1.42	1.36
2	D	601	55F	C2-N3	2.52	1.37	1.32
2	D	601	55F	C8-C9	2.50	1.43	1.39
2	E	601	55F	C10-C9	2.47	1.42	1.37
2	E	601	55F	C7-C8	2.47	1.42	1.36
2	E	601	55F	C8-C9	2.39	1.43	1.39
2	E	601	55F	C2-N3	2.32	1.37	1.32
2	E	601	55F	C16-N21	2.32	1.38	1.34
2	E	601	55F	C1-N6	2.31	1.37	1.32
3	D	14	PO4	P-O4	-2.21	1.48	1.54
2	A	601	55F	C16-N21	2.21	1.37	1.34
3	B	12	PO4	P-O2	-2.19	1.48	1.54
2	E	601	55F	C20-N21	2.15	1.37	1.34
2	A	601	55F	C5-C4	2.11	1.46	1.42
3	B	6	PO4	P-O3	-2.11	1.48	1.54
2	C	601	55F	C5-C4	2.09	1.46	1.42
2	B	601	55F	C8-C9	2.08	1.42	1.39
3	B	12	PO4	P-O3	-2.08	1.48	1.54
3	E	2	PO4	P-O2	-2.08	1.48	1.54
3	B	23	PO4	P-O4	-2.06	1.48	1.54
3	E	1	PO4	P-O3	-2.06	1.48	1.54
3	A	21	PO4	P-O4	-2.05	1.48	1.54
3	A	9	PO4	P-O3	-2.05	1.48	1.54
3	A	26	PO4	P-O3	-2.03	1.48	1.54
3	B	23	PO4	P-O3	-2.03	1.48	1.54
3	E	2	PO4	P-O3	-2.03	1.48	1.54
3	D	24	PO4	P-O4	-2.01	1.48	1.54
2	B	601	55F	C14-N13	-2.01	1.30	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	55F	O26-C25-N22	4.59	129.12	121.90
2	E	601	55F	O26-C25-N22	4.40	128.83	121.90
2	C	601	55F	O26-C25-N22	4.26	128.59	121.90
2	A	601	55F	O26-C25-N22	4.19	128.49	121.90
2	D	601	55F	O26-C25-N22	3.95	128.12	121.90
2	D	601	55F	C18-C19-C20	-2.93	118.81	122.15
2	C	601	55F	N15-C14-N13	-2.85	109.71	113.77
2	A	601	55F	C23-C20-C19	-2.72	120.14	122.88
2	A	601	55F	C19-C20-N21	2.69	122.05	118.47
2	B	601	55F	N15-C14-N13	-2.69	109.95	113.77
2	C	601	55F	C19-C20-N21	2.68	122.03	118.47
2	B	601	55F	C23-C20-C19	-2.64	120.22	122.88
2	E	601	55F	N15-C14-N13	-2.64	110.01	113.77
2	A	601	55F	N15-C14-N13	-2.63	110.02	113.77
2	B	601	55F	C27-C25-N22	-2.62	111.03	115.27
2	B	601	55F	C18-C19-C20	-2.61	119.17	122.15
2	E	601	55F	C27-C25-N22	-2.56	111.14	115.27
2	B	601	55F	C19-C20-N21	2.55	121.86	118.47
2	A	601	55F	C18-C19-C20	-2.55	119.24	122.15
2	D	601	55F	C27-C25-N22	-2.53	111.19	115.27
2	D	601	55F	C19-C20-N21	2.49	121.78	118.47
2	C	601	55F	C18-C19-C20	-2.48	119.33	122.15
2	E	601	55F	C19-C20-N21	2.45	121.72	118.47
2	A	601	55F	C27-C25-N22	-2.43	111.35	115.27
2	C	601	55F	C27-C25-N22	-2.40	111.39	115.27
2	D	601	55F	N15-C14-N13	-2.33	110.45	113.77
2	E	601	55F	C18-C19-C20	-2.33	119.49	122.15
2	E	601	55F	C23-C20-C19	-2.29	120.57	122.88
2	A	601	55F	C25-N22-C14	-2.28	122.80	127.56
2	D	601	55F	C10-C5-N6	2.24	120.58	118.01
2	D	601	55F	C25-N22-C14	-2.21	122.95	127.56
2	C	601	55F	C23-C20-C19	-2.17	120.69	122.88
2	D	601	55F	C12-C11-N15	-2.15	103.02	105.63
2	C	601	55F	C25-N22-C14	-2.03	123.33	127.56
2	E	601	55F	C25-N22-C14	-2.01	123.36	127.56
2	D	601	55F	C23-C20-C19	-2.01	120.85	122.88

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	55F	C11-C12-C16-C17
2	A	601	55F	C11-C12-C16-N21
2	A	601	55F	N13-C12-C16-C17
2	A	601	55F	N13-C12-C16-N21
2	A	601	55F	N15-C14-N22-C25
2	B	601	55F	C11-C12-C16-C17
2	B	601	55F	C11-C12-C16-N21
2	B	601	55F	N13-C12-C16-C17
2	B	601	55F	N13-C12-C16-N21
2	C	601	55F	C11-C12-C16-C17
2	C	601	55F	C11-C12-C16-N21
2	C	601	55F	N13-C12-C16-C17
2	C	601	55F	N13-C12-C16-N21
2	C	601	55F	N13-C14-N22-C25
2	C	601	55F	N15-C14-N22-C25
2	D	601	55F	C11-C12-C16-C17
2	D	601	55F	C11-C12-C16-N21
2	D	601	55F	N13-C12-C16-C17
2	D	601	55F	N13-C12-C16-N21
2	D	601	55F	N13-C14-N22-C25
2	D	601	55F	N15-C14-N22-C25
2	E	601	55F	C11-C12-C16-C17
2	E	601	55F	C11-C12-C16-N21
2	E	601	55F	N13-C12-C16-C17
2	E	601	55F	N13-C12-C16-N21
2	A	601	55F	N13-C14-N22-C25

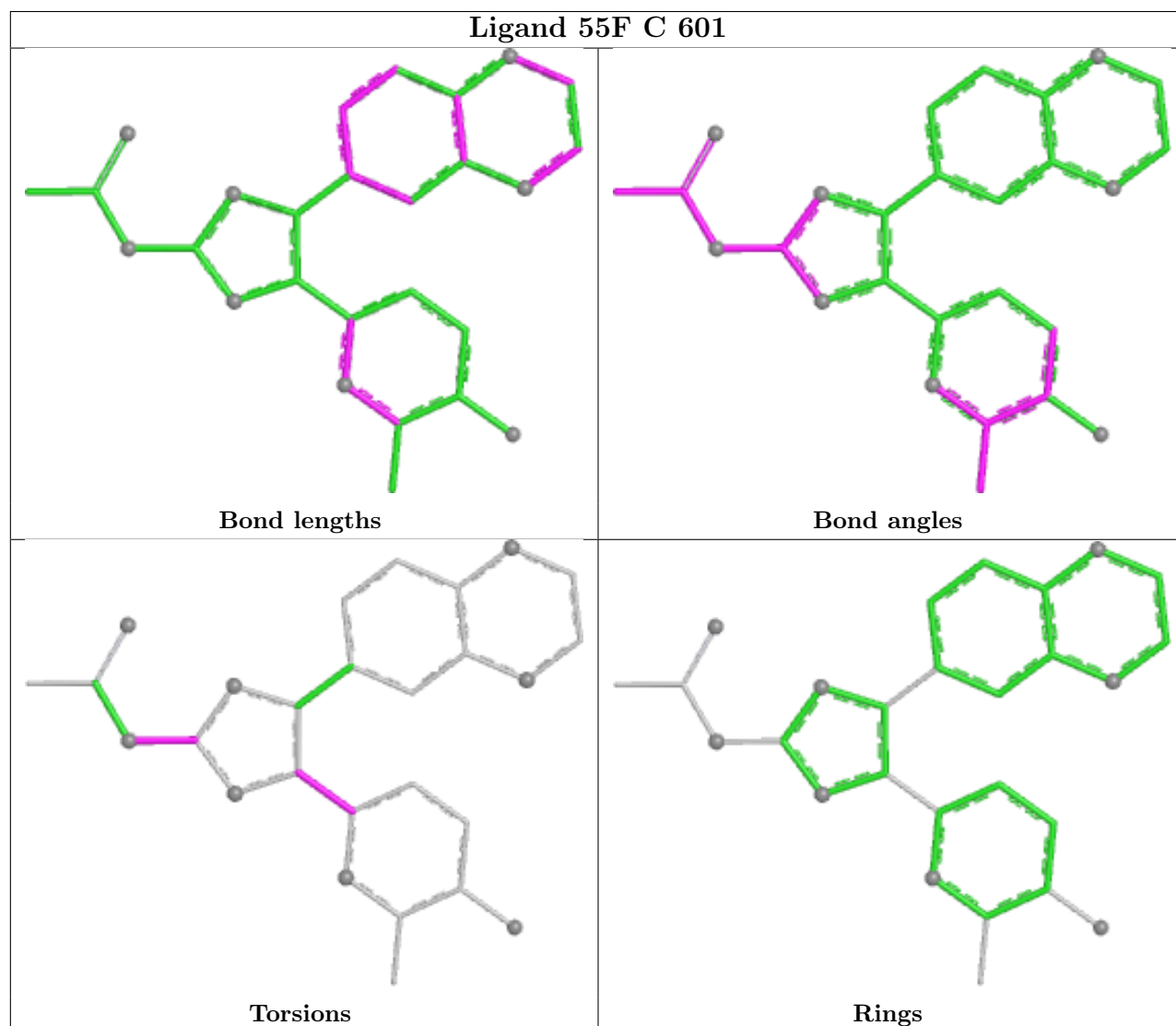
There are no ring outliers.

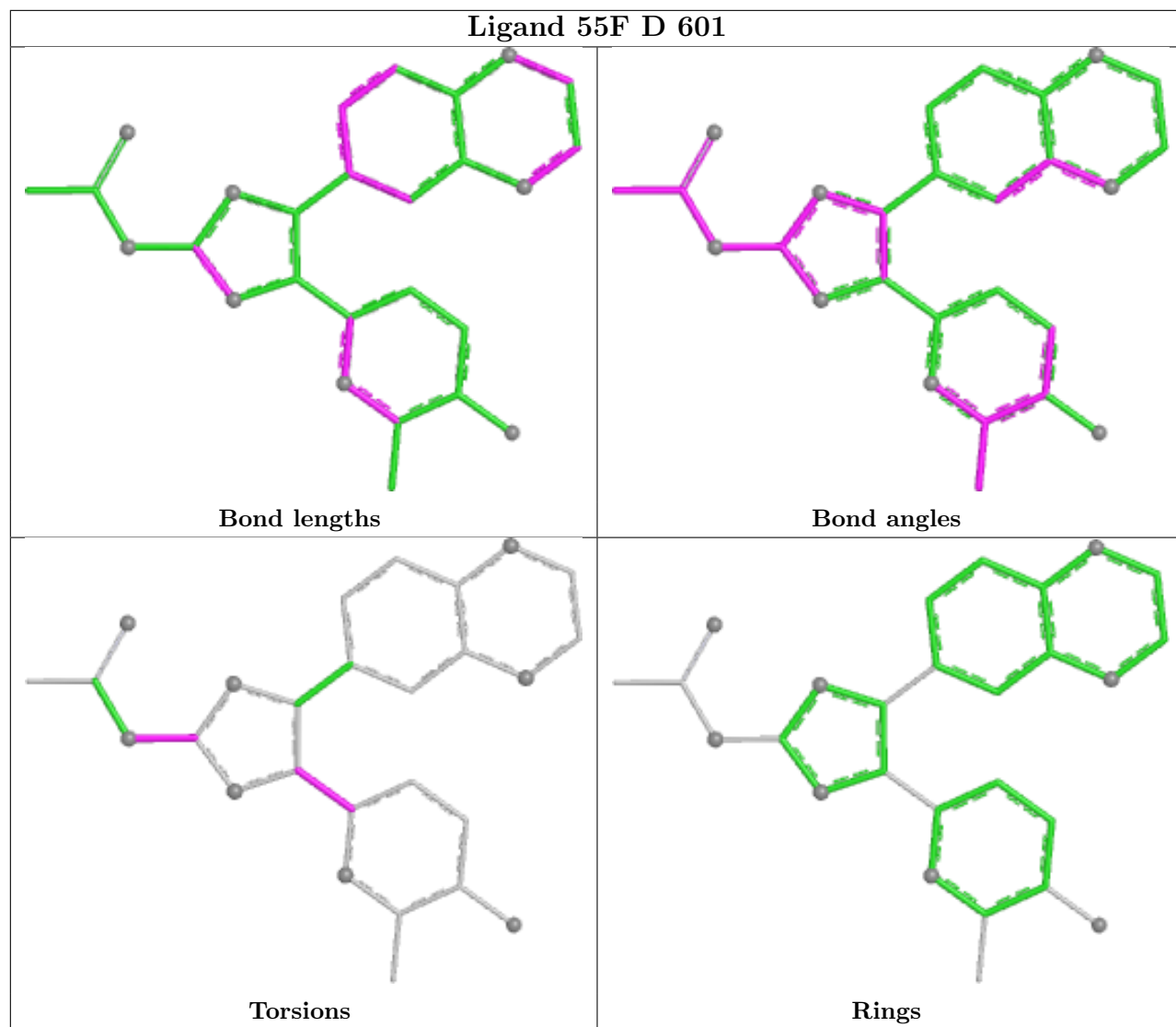
8 monomers are involved in 12 short contacts:

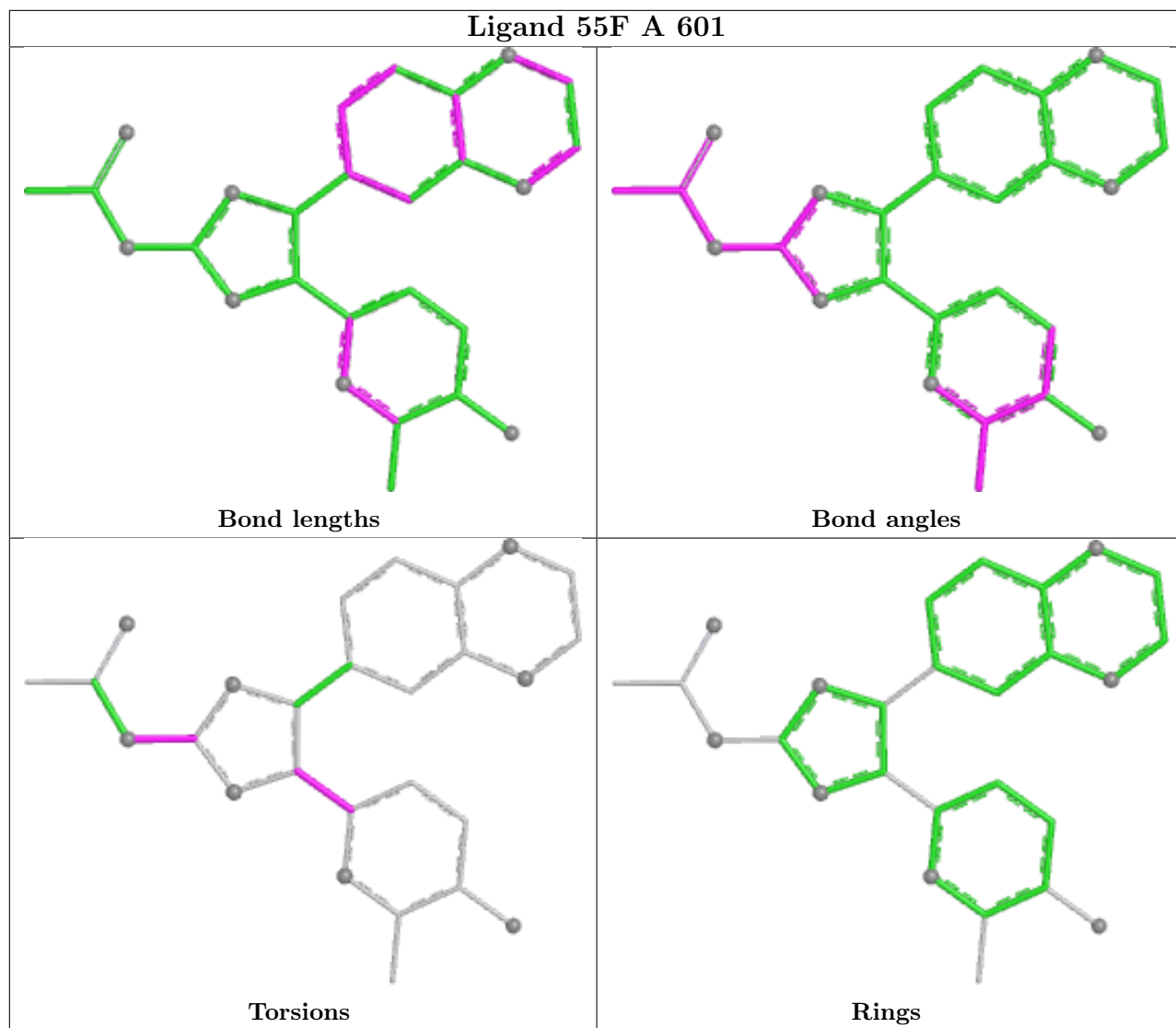
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	55F	1	0
3	A	9	PO4	2	0
3	B	23	PO4	1	0
3	E	2	PO4	2	0
2	A	601	55F	1	0
3	D	13	PO4	2	0
2	B	601	55F	2	0
2	E	601	55F	1	0

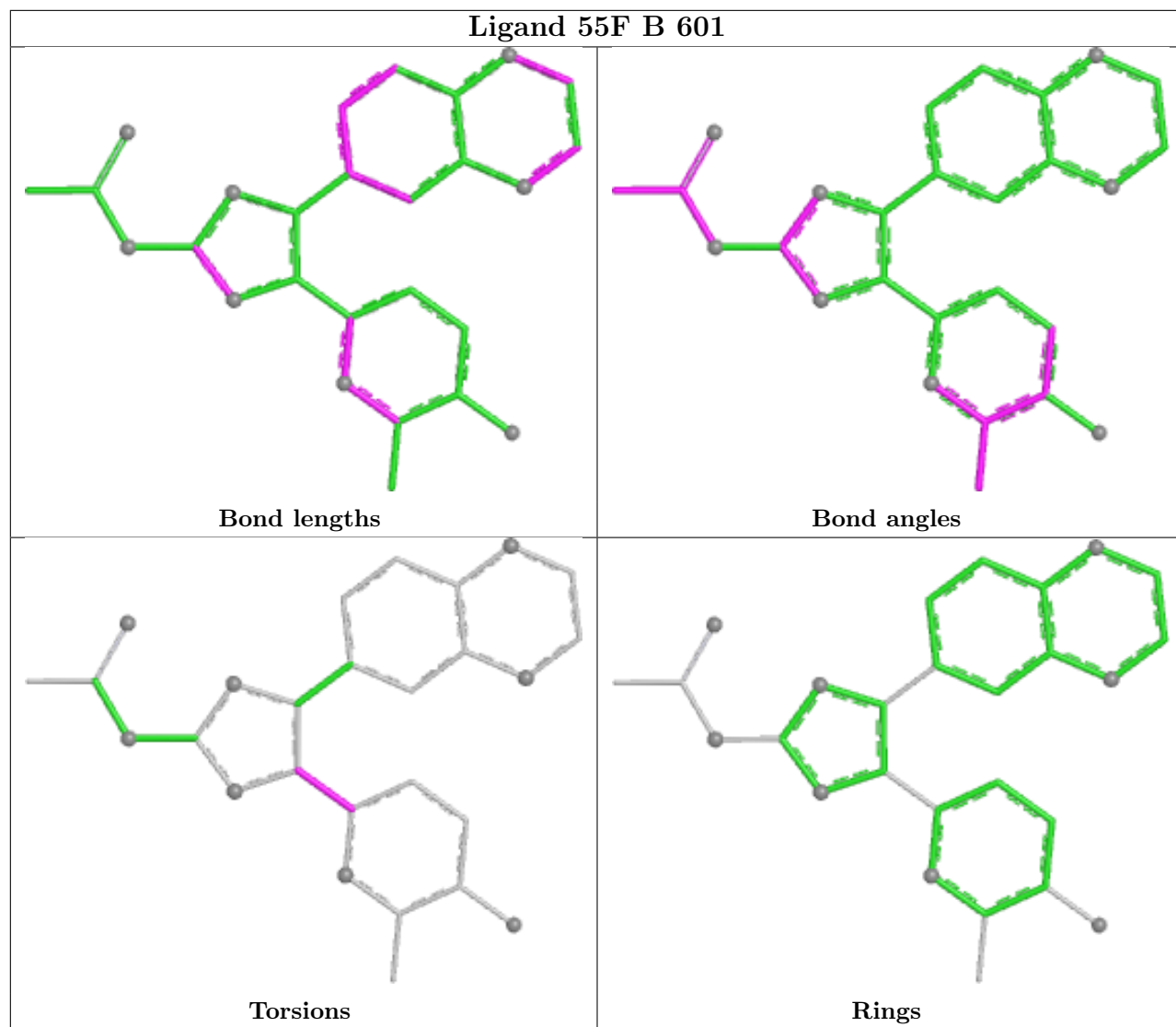
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

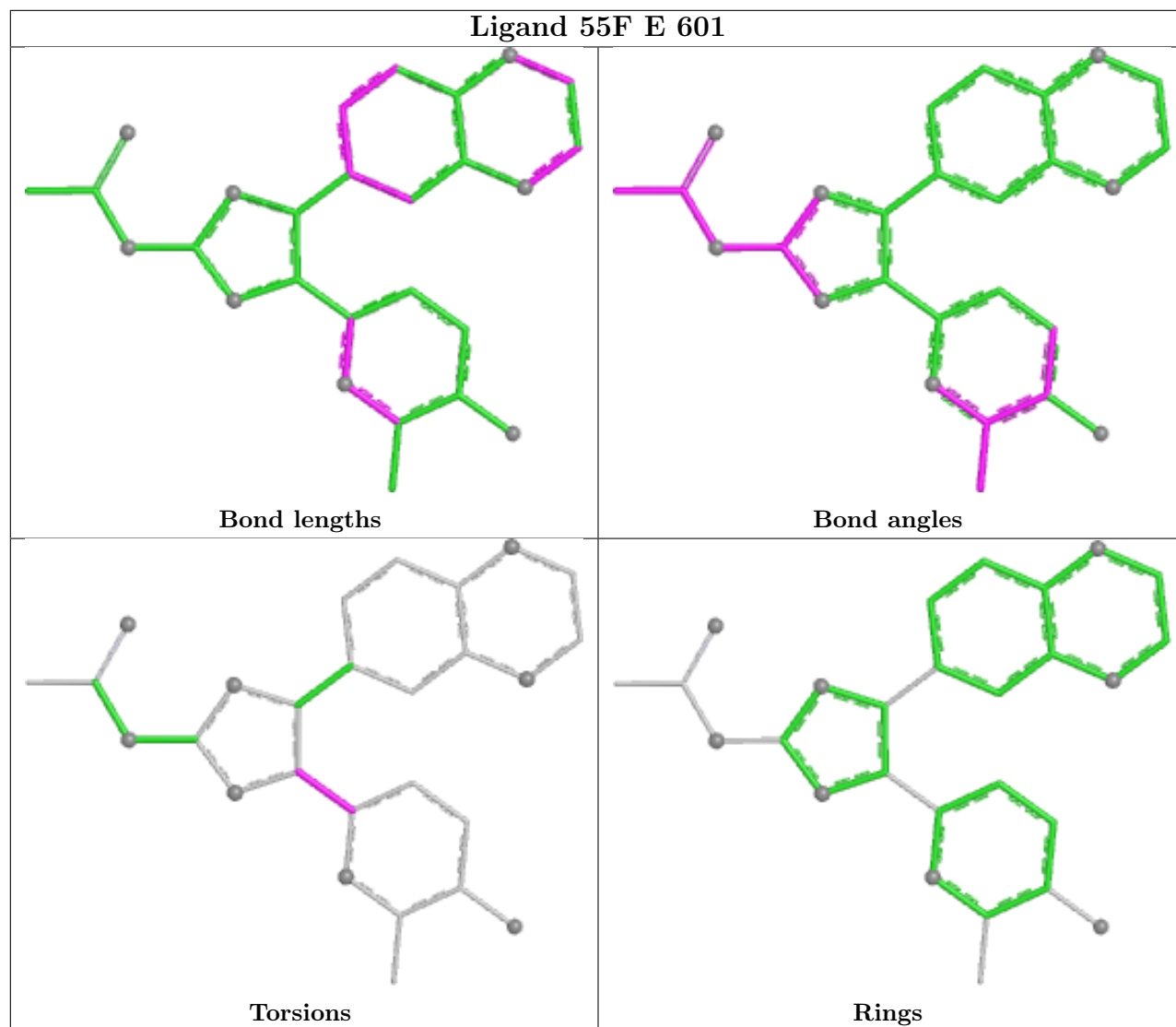
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/342 (95%)	0.05	4 (1%) 76 63	31, 89, 131, 142	0
1	B	324/342 (94%)	-0.36	0 100 100	27, 51, 84, 105	0
1	C	330/342 (96%)	0.47	21 (6%) 25 19	28, 101, 138, 144	0
1	D	330/342 (96%)	-0.23	4 (1%) 76 63	31, 58, 97, 109	0
1	E	330/342 (96%)	-0.35	4 (1%) 76 63	26, 51, 86, 109	0
All	All	1642/1710 (96%)	-0.08	33 (2%) 65 48	26, 63, 128, 144	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	368	ALA	5.8
1	E	369	PRO	5.5
1	C	427	PRO	4.1
1	C	491	THR	4.1
1	C	495	LEU	3.8
1	C	431	LEU	3.6
1	E	500	GLY	3.3
1	C	500	GLY	3.3
1	C	405	GLY	3.2
1	C	496	SER	3.1
1	C	426	LEU	3.0
1	C	466	VAL	2.7
1	C	492	LEU	2.7
1	D	500	GLY	2.6
1	D	446	CYS	2.6
1	A	367	ILE	2.6
1	C	408	PHE	2.6
1	D	420	ILE	2.5
1	C	378	TYR	2.5
1	C	450	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	488	ILE	2.5
1	C	418	GLY	2.5
1	C	369	PRO	2.4
1	C	338	ASN	2.4
1	C	367	ILE	2.3
1	C	455	PRO	2.2
1	A	257	GLU	2.2
1	C	477	ALA	2.1
1	A	464	LEU	2.0
1	C	420	ILE	2.0
1	D	236	SER	2.0
1	E	191	SER	2.0
1	A	438	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	9	5/5	0.77	0.09	103,103,104,104	0
3	PO4	D	14	5/5	0.84	0.28	21,22,22,23	5
3	PO4	C	10	5/5	0.86	0.07	103,104,104,105	0
3	PO4	B	23	5/5	0.86	0.34	31,31,32,32	5
3	PO4	B	12	5/5	0.88	0.28	20,21,22,23	5
3	PO4	A	21	5/5	0.91	0.14	36,36,37,38	5
3	PO4	D	24	5/5	0.91	0.30	29,29,31,31	5
3	PO4	E	22	5/5	0.91	0.26	18,18,20,20	5
3	PO4	A	26	5/5	0.92	0.17	48,48,48,49	5
3	PO4	B	6	5/5	0.92	0.08	60,63,63,65	0

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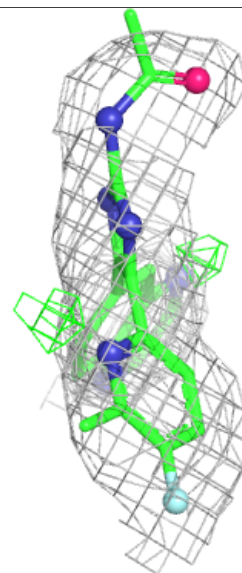
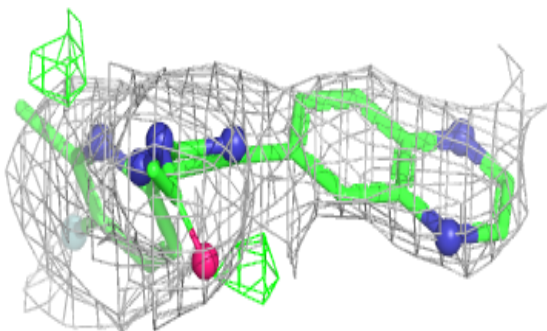
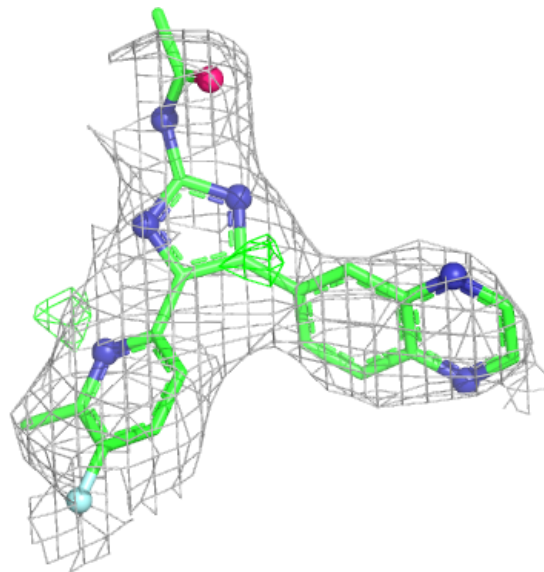
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	E	1	5/5	0.93	0.08	89,89,90,90	0
3	PO4	D	13	5/5	0.93	0.09	82,82,83,84	0
2	55F	C	601	27/27	0.94	0.11	73,79,81,81	0
3	PO4	E	2	5/5	0.94	0.21	7,8,8,9	5
2	55F	D	601	27/27	0.94	0.10	48,49,58,61	0
2	55F	B	601	27/27	0.96	0.09	29,39,49,52	0
2	55F	E	601	27/27	0.96	0.10	36,40,59,62	0
2	55F	A	601	27/27	0.96	0.09	46,53,65,67	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.

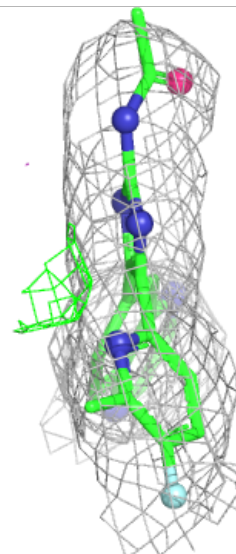
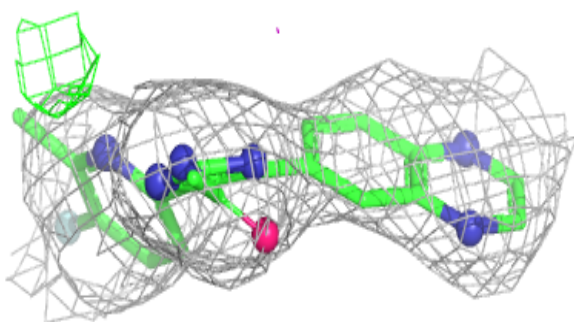
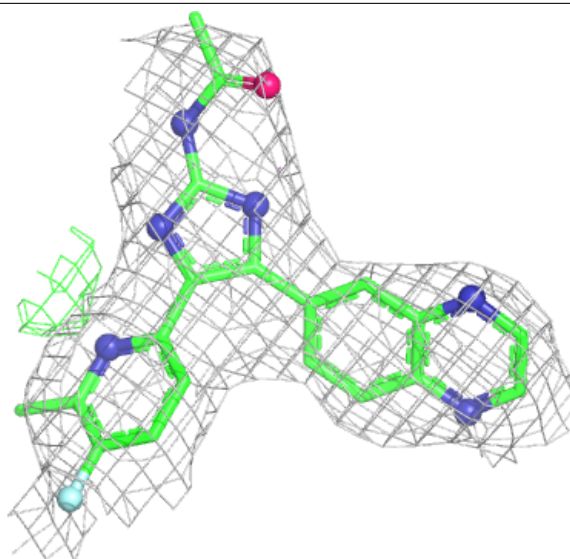
Electron density around 55F C 601:

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



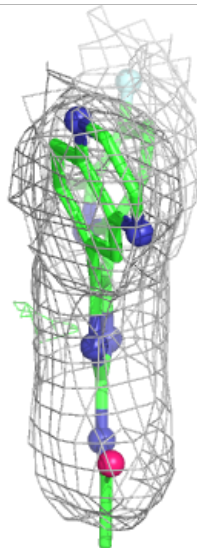
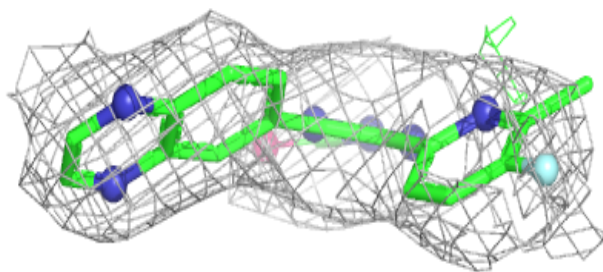
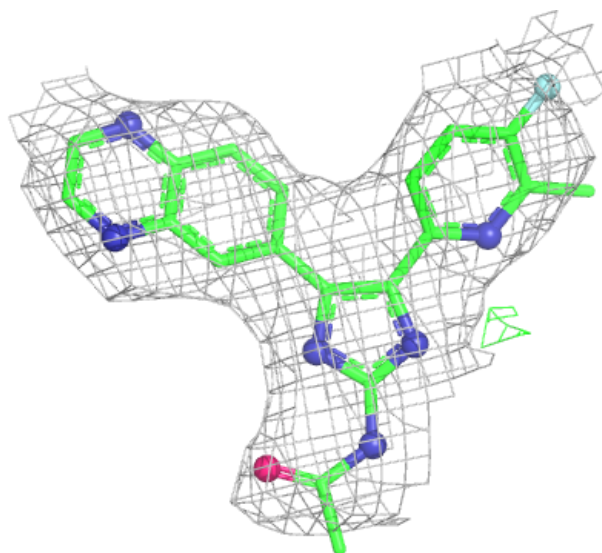
Electron density around 55F D 601:

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



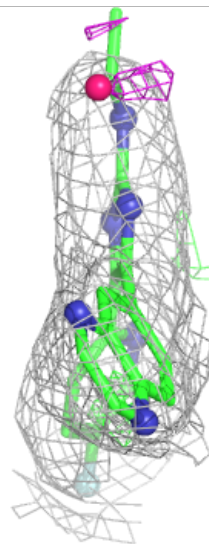
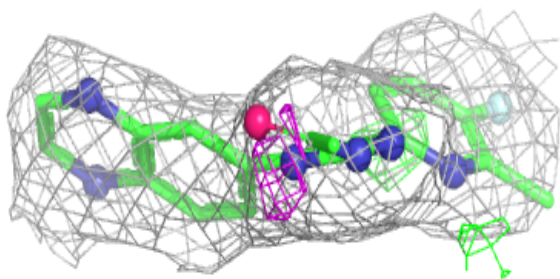
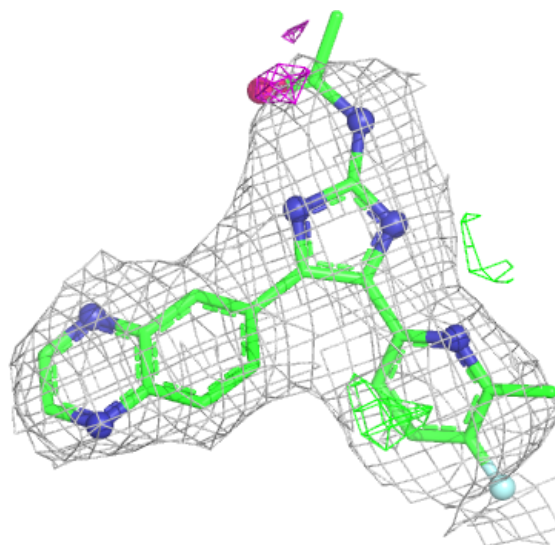
Electron density around 55F B 601:

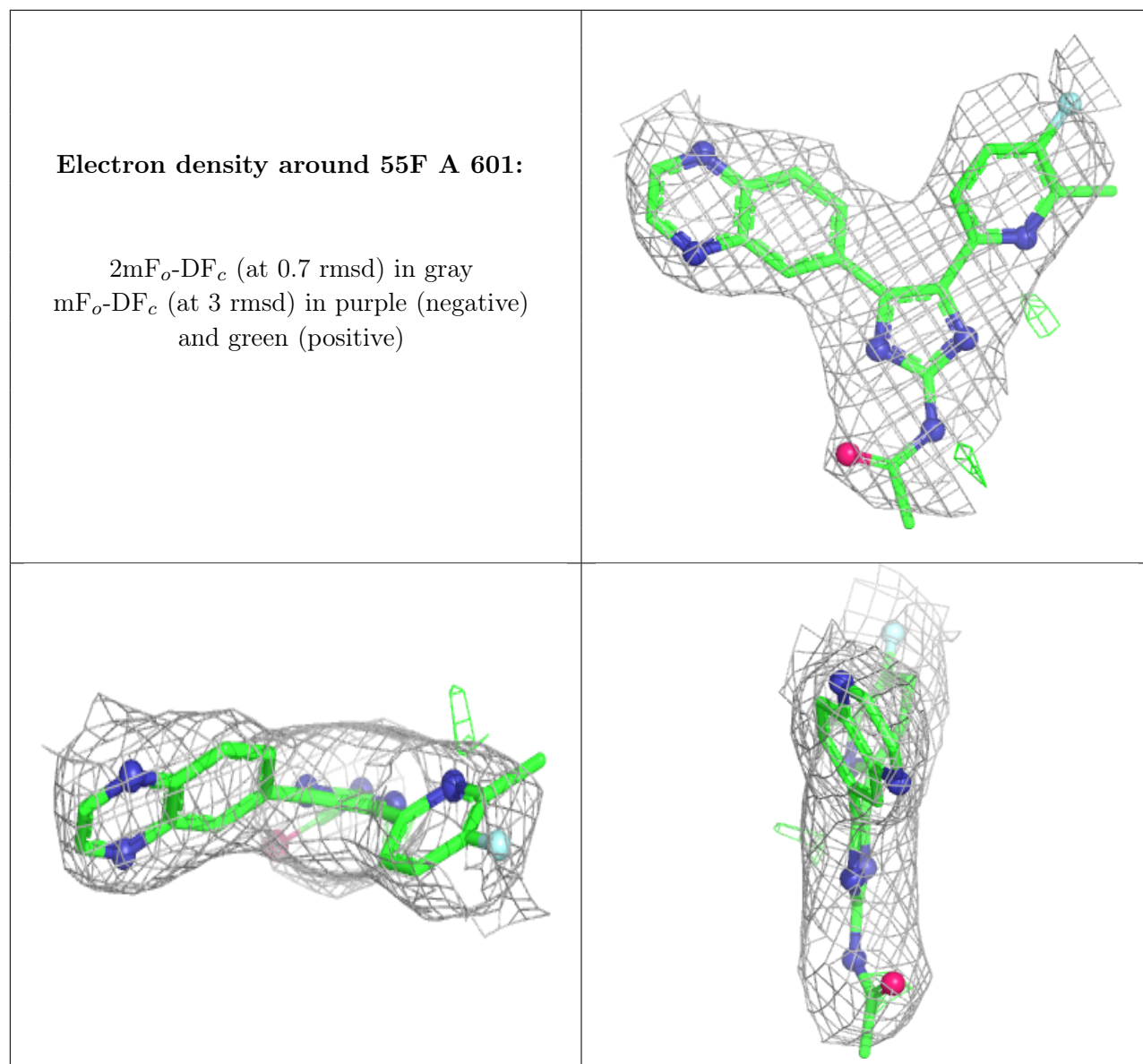
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 55F E 601:

$2mF_o-DF_c$ (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.