



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:57 PM UTC

PDB ID : 6BAP / pdb_00006bap
Title : Stigmatella aurantiaca bacterial phytochrome PAS-GAF-PHY, T289H mutant
Authors : Schmidt, M.; Stojkovic, E.
Deposited on : 2017-10-14
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

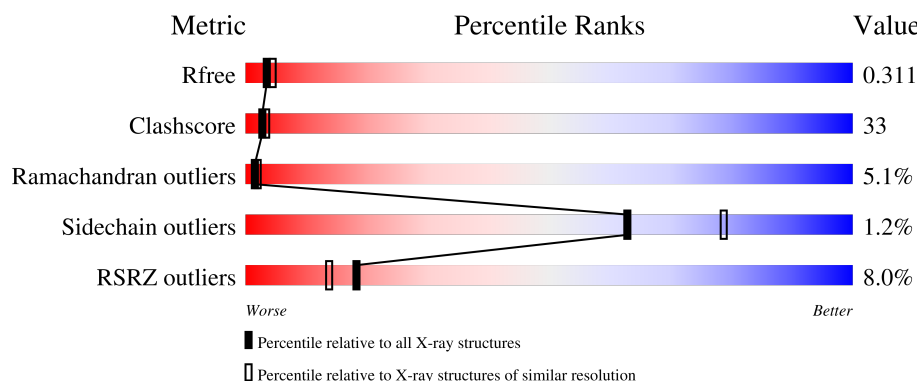
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	515	
1	B	515	
1	C	515	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12158 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.

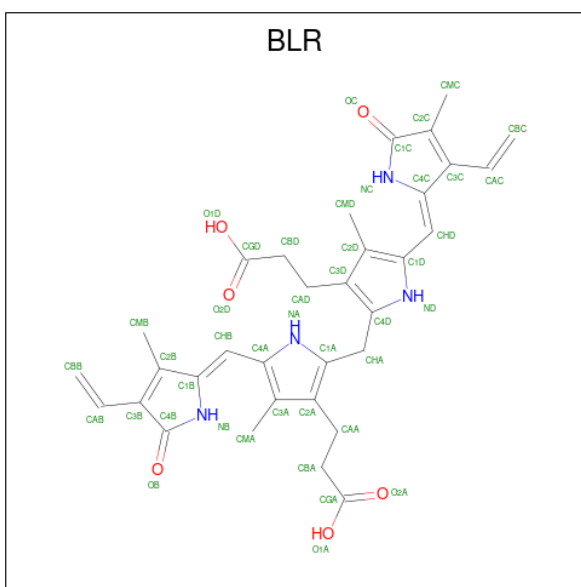
- Molecule 1 is a protein called Photoreceptor-histidine kinase BphP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3982	2513	726	730	13			
1	B	505	Total	C	N	O	S	0	0	0
			3982	2513	726	730	13			
1	C	500	Total	C	N	O	S	0	0	0
			3941	2488	720	720	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	HIS	THR	engineered mutation	UNP Q097N3
B	289	HIS	THR	engineered mutation	UNP Q097N3
C	289	HIS	THR	engineered mutation	UNP Q097N3

- Molecule 2 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (CCD ID: BLR) (formula: C₃₃H₃₆N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0
2	C	1	Total 43	C 33	N 4	O 6	0	0

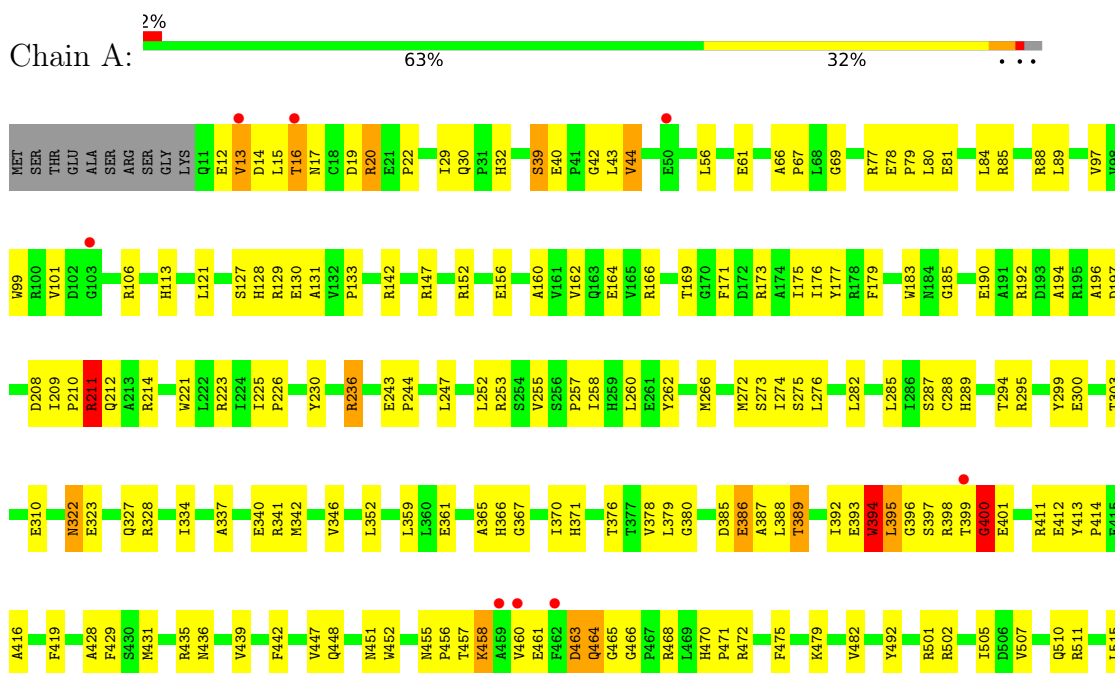
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	42	Total O 42 42	0	0
3	C	36	Total O 36 36	0	0

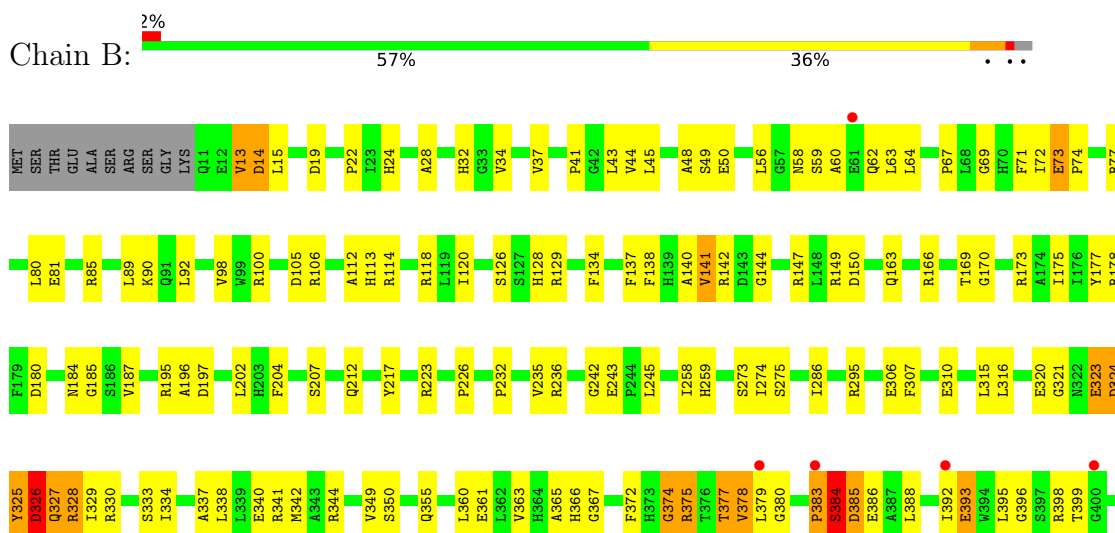
3 Residue-property plots

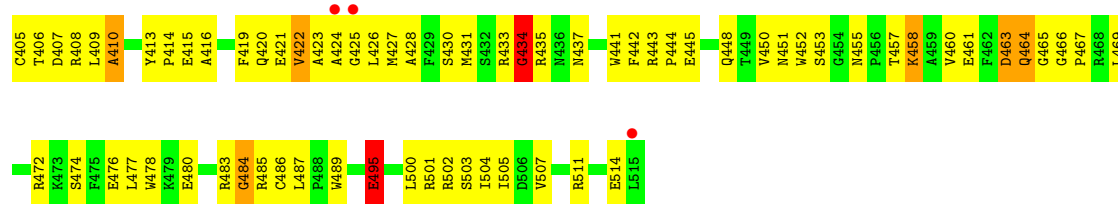
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photoreceptor-histidine kinase BphP

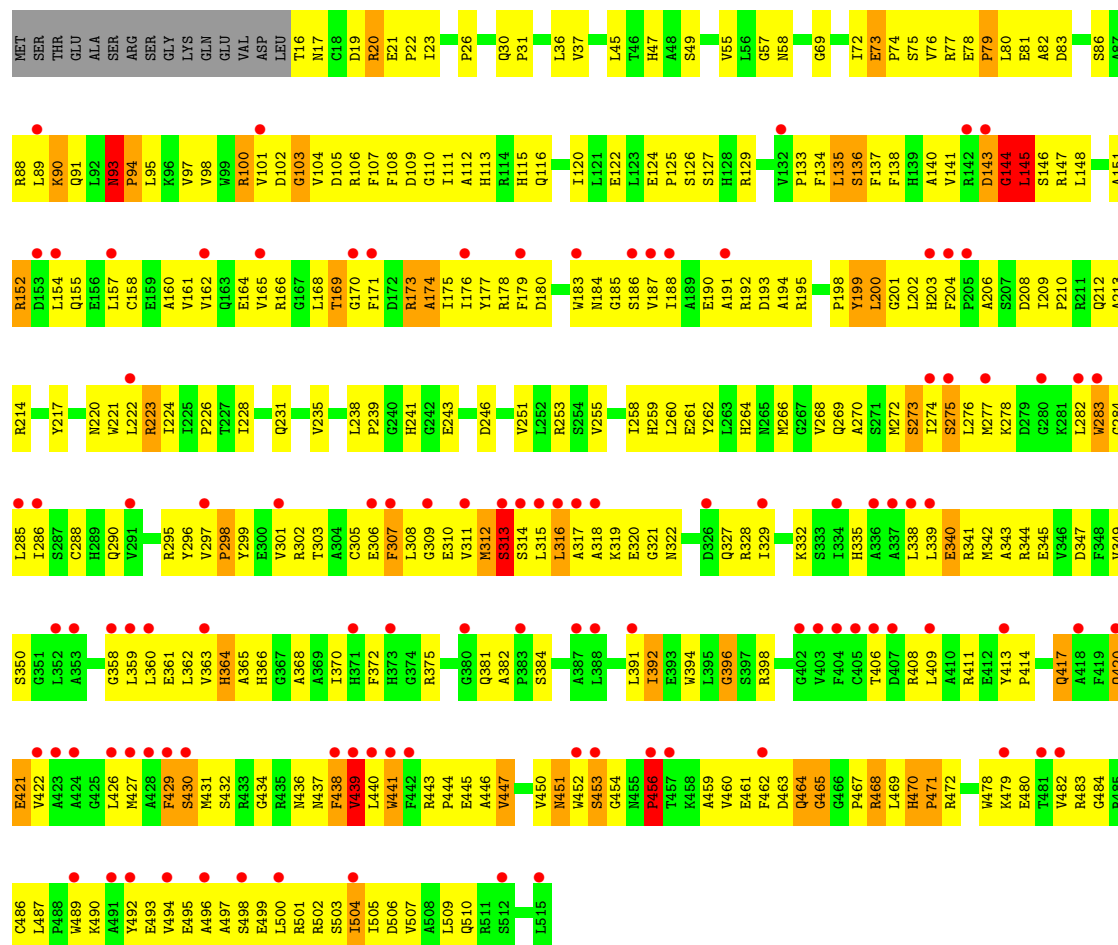


• Molecule 1: Photoreceptor-histidine kinase BphP





● Molecule 1: Photoreceptor-histidine kinase BphP



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.31Å 83.31Å 475.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.28 – 2.65 40.28 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.28-2.65) 98.8 (40.28-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.241 , 0.315 0.243 , 0.311	Depositor DCC
R_{free} test set	3051 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12158	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: BLR

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	0.56	3/4075 (0.1%)	0.80	8/5529 (0.1%)
1	B	0.52	3/4075 (0.1%)	0.82	10/5529 (0.2%)
1	C	0.91	12/4034 (0.3%)	0.96	15/5473 (0.3%)
All	All	0.69	18/12184 (0.1%)	0.86	33/16531 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	14
All	All	0	19

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	PRO	N-CD	-34.71	0.99	1.47
1	C	74	PRO	N-CD	-17.37	1.23	1.47
1	C	173	ARG	NE-CZ	-9.79	1.22	1.33
1	C	173	ARG	CZ-NH2	-9.29	1.21	1.33
1	C	100	ARG	NE-CZ	-9.28	1.22	1.33
1	C	483	ARG	NE-CZ	-9.17	1.23	1.33
1	C	483	ARG	CZ-NH2	-8.22	1.22	1.33
1	C	483	ARG	CD-NE	-8.11	1.34	1.46
1	C	100	ARG	CZ-NH2	-7.99	1.23	1.33
1	A	236	ARG	NE-CZ	-7.74	1.24	1.33
1	C	100	ARG	CZ-NH1	-7.52	1.22	1.32
1	C	100	ARG	CD-NE	-6.55	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ARG	CZ-NH1	-6.31	1.24	1.32
1	C	483	ARG	CZ-NH1	-6.12	1.24	1.32
1	B	458	LYS	CD-CE	-5.79	1.35	1.52
1	B	495	GLU	CD-OE1	-5.38	1.15	1.25
1	B	410	ALA	CA-C	5.35	1.59	1.52
1	A	211	ARG	CZ-NH2	-5.29	1.26	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	TYR	C-N-CD	-10.37	97.78	120.60
1	A	394	TRP	CA-CB-CG	10.21	133.01	113.60
1	C	223	ARG	CG-CD-NE	-8.89	92.44	112.00
1	B	434	GLY	CA-C-N	8.48	135.84	122.61
1	B	434	GLY	C-N-CA	8.48	135.84	122.61
1	C	413	TYR	CA-C-N	7.86	145.87	127.00
1	C	413	TYR	C-N-CA	7.86	145.87	127.00
1	B	13	VAL	CA-C-N	7.18	134.63	121.70
1	B	13	VAL	C-N-CA	7.18	134.63	121.70
1	C	298	PRO	N-CA-CB	-7.10	95.80	103.25
1	B	326	ASP	N-CA-C	-6.76	97.58	109.06
1	A	13	VAL	CA-C-N	6.45	133.31	121.70
1	A	13	VAL	C-N-CA	6.45	133.31	121.70
1	A	20	ARG	CG-CD-NE	6.27	125.80	112.00
1	B	374	GLY	CA-C-N	6.03	132.56	121.70
1	B	374	GLY	C-N-CA	6.03	132.56	121.70
1	C	298	PRO	CB-CG-CD	-6.00	86.89	106.10
1	C	223	ARG	CB-CA-C	-5.94	97.62	111.09
1	A	464	GLN	N-CA-C	5.93	118.70	111.82
1	B	327	GLN	CA-CB-CG	-5.65	102.81	114.10
1	C	456	PRO	CA-N-CD	-5.64	104.11	112.00
1	C	145	LEU	CB-CG-CD1	-5.56	94.02	110.70
1	C	441	TRP	CA-CB-CG	-5.53	103.09	113.60
1	C	451	ASN	N-CA-C	5.45	121.77	112.99
1	C	144	GLY	N-CA-C	-5.35	100.50	113.18
1	C	396	GLY	CA-C-N	5.35	131.32	121.70
1	C	396	GLY	C-N-CA	5.35	131.32	121.70
1	C	316	LEU	CD1-CG-CD2	5.27	122.39	110.80
1	A	211	ARG	CG-CD-NE	5.25	123.55	112.00
1	A	397	SER	CA-C-N	5.19	131.05	121.70
1	A	397	SER	C-N-CA	5.19	131.05	121.70
1	B	327	GLN	N-CA-C	5.18	125.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	GLN	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	GLY	Peptide
1	B	325	TYR	Peptide
1	B	326	ASP	Peptide
1	B	393	GLU	Peptide
1	B	422	VAL	Peptide
1	C	135	LEU	Peptide
1	C	143	ASP	Peptide
1	C	144	GLY	Peptide
1	C	199	TYR	Peptide
1	C	222	LEU	Peptide
1	C	273	SER	Peptide
1	C	275	SER	Peptide
1	C	313	SER	Peptide
1	C	420	GLN	Peptide
1	C	430	SER	Peptide
1	C	438	PHE	Peptide
1	C	439	VAL	Peptide
1	C	504	ILE	Peptide
1	C	93	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	3925	183	0
1	B	3982	0	3925	200	0
1	C	3941	0	3886	433	0
2	A	43	0	32	4	0
2	B	43	0	32	3	0
2	C	43	0	33	14	0
3	A	46	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	0	5	0
3	C	36	0	0	18	0
All	All	12158	0	11833	789	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 33.

All (789) 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:142:ARG:NH1	1:B:307:PHE:CA	1.72	1.51
1:A:142:ARG:NH1	1:B:307:PHE:HA	1.19	1.44
1:C:429:PHE:O	1:C:501:ARG:NH1	1.65	1.29
1:A:142:ARG:HH11	1:B:307:PHE:CB	1.54	1.19
1:C:429:PHE:C	1:C:501:ARG:NH1	2.03	1.15
1:C:154:LEU:HD21	1:C:155:GLN:NE2	1.65	1.12
1:C:429:PHE:C	1:C:501:ARG:HH11	1.56	1.11
1:A:142:ARG:HH12	1:B:307:PHE:CA	1.39	1.11
1:C:37:VAL:HG12	1:C:120:ILE:HG22	1.30	1.09
1:C:202:LEU:HD21	1:C:452:TRP:HA	1.31	1.09
1:A:142:ARG:HH22	1:B:306:GLU:HG2	1.08	1.08
1:C:278:LYS:CD	1:C:316:LEU:HD22	1.83	1.08
1:C:278:LYS:HD2	1:C:316:LEU:CD2	1.87	1.04
1:C:297:VAL:HG22	1:C:301:VAL:HG13	1.40	1.04
1:A:142:ARG:HH11	1:B:307:PHE:HB2	1.22	1.04
1:C:497:ALA:HB1	1:C:501:ARG:HH22	1.13	1.02
1:C:497:ALA:CB	1:C:501:ARG:HH22	1.46	1.02
1:C:154:LEU:HD21	1:C:155:GLN:HE22	1.19	0.98
1:C:278:LYS:HD2	1:C:316:LEU:HD22	1.00	0.98
1:C:154:LEU:CD2	1:C:155:GLN:NE2	2.26	0.98
1:A:142:ARG:NH1	1:B:307:PHE:CB	2.19	0.98
1:A:401:GLU:OE2	1:A:501:ARG:NH2	1.97	0.98
1:C:168:LEU:HD11	1:C:305:CYS:SG	2.03	0.97
1:C:88:ARG:HB3	1:C:90:LYS:HE3	1.46	0.97
1:A:142:ARG:NH2	1:B:306:GLU:HG2	1.80	0.97
1:C:73:GLU:HB3	1:C:100:ARG:HG3	1.42	0.97
1:C:151:ALA:HB3	1:C:157:LEU:CD1	1.95	0.96
1:B:425:GLY:H	1:B:443:ARG:H	0.97	0.95
1:C:100:ARG:NH1	1:C:105:ASP:OD2	1.98	0.95
1:C:202:LEU:HD23	1:C:451:ASN:ND2	1.82	0.95
1:B:430:SER:HB2	1:B:433:ARG:HH12	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ALA:HB1	1:C:501:ARG:NH2	1.81	0.94
1:B:13:VAL:HA	1:B:14:ASP:HB2	1.49	0.94
1:B:324:ASP:OD1	1:B:328:ARG:NH2	2.00	0.94
1:C:497:ALA:CB	1:C:501:ARG:NH2	2.31	0.94
1:C:408:ARG:NH2	1:C:421:GLU:OE1	2.02	0.92
1:C:297:VAL:CG2	1:C:301:VAL:HG13	1.99	0.92
1:C:213:ALA:HB1	1:C:217:TYR:HE2	1.32	0.92
1:C:175:ILE:HD13	1:C:187:VAL:HG13	1.51	0.92
1:C:274:ILE:HD12	1:C:306:GLU:HA	1.49	0.92
1:A:13:VAL:HA	1:A:14:ASP:HB2	1.50	0.91
1:C:456:PRO:HD2	1:C:478:TRP:CH2	2.06	0.90
1:B:169:THR:O	1:B:295:ARG:NH2	2.04	0.90
1:A:142:ARG:NH1	1:B:307:PHE:N	2.18	0.90
1:C:427:MET:HE1	1:C:494:VAL:HA	1.55	0.89
1:C:73:GLU:OE1	1:C:75:SER:N	2.06	0.89
1:A:43:LEU:HG	1:A:44:VAL:HG12	1.55	0.88
1:C:154:LEU:HD23	1:C:155:GLN:CD	1.98	0.88
1:C:202:LEU:HD13	1:C:202:LEU:C	1.99	0.87
1:B:41:PRO:O	1:B:85:ARG:NH1	2.07	0.86
1:C:171:PHE:HE2	1:C:295:ARG:HG2	1.41	0.86
1:C:298:PRO:HD2	1:C:301:VAL:CG1	2.06	0.86
1:C:321:GLY:HA2	1:C:492:TYR:HE1	1.41	0.85
1:A:142:ARG:HH12	1:B:307:PHE:N	1.72	0.85
1:C:174:ALA:HB3	1:C:191:ALA:HB3	1.60	0.84
1:A:398:ARG:HG2	1:A:399:THR:H	1.42	0.84
1:A:142:ARG:HH11	1:B:307:PHE:CA	1.64	0.83
1:C:202:LEU:HD21	1:C:452:TRP:CA	2.09	0.83
1:C:157:LEU:HD21	3:C:706:HOH:O	1.78	0.82
1:A:69:GLY:O	1:A:77:ARG:NH1	2.12	0.82
1:B:430:SER:HB2	1:B:433:ARG:NH1	1.95	0.82
1:C:368:ALA:HA	1:C:440:LEU:HD21	1.59	0.82
1:A:42:GLY:HA3	1:A:85:ARG:HH21	1.43	0.82
1:A:192:ARG:NH2	1:C:81:GLU:OE2	2.13	0.82
1:B:330:ARG:NH1	1:B:361:GLU:OE1	2.12	0.82
1:C:37:VAL:HG12	1:C:120:ILE:CG2	2.10	0.81
1:C:276:LEU:HD11	1:C:312:MET:HG2	1.61	0.81
1:A:322:ASN:ND2	1:A:322:ASN:O	2.13	0.81
1:C:202:LEU:HD23	1:C:451:ASN:CG	2.05	0.81
1:C:202:LEU:HB2	1:C:451:ASN:ND2	1.97	0.80
1:B:425:GLY:H	1:B:443:ARG:N	1.79	0.80
1:B:453:SER:O	1:B:472:ARG:NH2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD23	1:C:155:GLN:OE1	1.82	0.80
1:A:192:ARG:NH1	1:A:196:ALA:O	2.15	0.79
1:C:161:VAL:O	1:C:165:VAL:N	2.13	0.79
1:A:142:ARG:HH12	1:B:307:PHE:HA	0.81	0.79
1:C:187:VAL:HB	1:C:202:LEU:H	1.47	0.78
1:C:452:TRP:HB2	1:C:478:TRP:CH2	2.17	0.78
1:C:113:HIS:CD2	1:C:120:ILE:HD11	2.18	0.78
1:C:213:ALA:HB1	1:C:217:TYR:CE2	2.18	0.78
1:B:410:ALA:HA	1:B:414:PRO:HA	1.67	0.77
1:A:142:ARG:NH1	1:B:307:PHE:HB2	1.89	0.77
1:C:164:GLU:O	1:C:168:LEU:HD23	1.84	0.77
1:B:374:GLY:HA3	1:B:375:ARG:HB2	1.67	0.77
1:C:214:ARG:HA	1:C:217:TYR:HD2	1.50	0.77
1:A:194:ALA:HB3	1:C:78:GLU:HG2	1.67	0.77
1:C:359:LEU:HD11	1:C:441:TRP:CE2	2.20	0.77
1:C:210:PRO:HG3	2:C:601:BLR:H24	1.65	0.76
1:A:502:ARG:HA	1:A:505:ILE:HD12	1.66	0.76
1:C:107:PHE:HB3	1:C:127:SER:HB3	1.65	0.76
1:C:154:LEU:CD2	1:C:155:GLN:CD	2.57	0.76
1:C:171:PHE:CE2	1:C:295:ARG:HG2	2.21	0.76
1:C:278:LYS:HG2	1:C:283:TRP:HB2	1.67	0.76
1:C:312:MET:SD	1:C:313:SER:N	2.59	0.76
1:A:197:ASP:OD2	1:C:77:ARG:NH2	2.19	0.75
1:B:326:ASP:OD1	1:B:329:ILE:HB	1.87	0.75
1:B:408:ARG:NH1	3:B:701:HOH:O	2.18	0.75
1:C:429:PHE:N	1:C:501:ARG:HH12	1.85	0.75
1:C:16:THR:N	1:C:19:ASP:OD2	2.20	0.74
1:C:161:VAL:O	1:C:165:VAL:HG13	1.86	0.74
1:C:253:ARG:NH1	2:C:601:BLR:O2D	2.18	0.74
1:A:175:ILE:HG22	1:A:190:GLU:HB2	1.68	0.74
1:C:312:MET:O	1:C:314:SER:N	2.19	0.74
1:B:327:GLN:O	1:B:329:ILE:N	2.20	0.74
1:A:142:ARG:NH2	1:B:310:GLU:OE2	2.21	0.73
1:A:398:ARG:HG2	1:A:399:THR:N	2.03	0.73
1:B:392:ILE:HD12	1:B:393:GLU:HG3	1.70	0.73
1:C:137:PHE:O	3:C:701:HOH:O	2.05	0.73
1:C:168:LEU:CD1	1:C:305:CYS:SG	2.77	0.73
1:B:478:TRP:HZ3	1:B:480:GLU:HB2	1.54	0.72
1:C:208:ASP:OD2	1:C:472:ARG:NH1	2.23	0.72
1:C:430:SER:HA	1:C:501:ARG:CD	2.19	0.72
1:C:129:ARG:NH2	1:C:296:TYR:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ALA:HB3	1:C:157:LEU:HD12	1.70	0.72
1:C:175:ILE:HD13	1:C:187:VAL:CG1	2.19	0.72
1:C:202:LEU:HD13	1:C:202:LEU:O	1.90	0.72
1:A:398:ARG:HD3	1:A:435:ARG:HH12	1.54	0.72
1:C:446:ALA:HB2	1:C:487:LEU:HG	1.71	0.72
1:C:49:SER:HA	1:C:235:VAL:HA	1.72	0.72
1:B:474:SER:OG	1:B:476:GLU:OE1	2.05	0.72
1:C:187:VAL:HG21	1:C:202:LEU:O	1.90	0.71
1:B:178:ARG:NH2	1:B:320:GLU:OE2	2.23	0.71
1:C:113:HIS:NE2	1:C:120:ILE:HD11	2.05	0.71
1:C:422:VAL:HG11	1:C:486:CYS:HB2	1.72	0.71
1:A:223:ARG:NH2	1:A:273:SER:OG	2.22	0.71
1:C:201:GLY:O	1:C:451:ASN:ND2	2.19	0.71
1:C:266:MET:HE2	1:C:268:VAL:HG21	1.73	0.71
1:B:89:LEU:HA	1:B:92:LEU:HD12	1.71	0.70
1:C:192:ARG:CZ	1:C:198:PRO:HG3	2.21	0.70
1:C:321:GLY:HA2	1:C:492:TYR:CE1	2.26	0.70
1:C:447:VAL:HB	1:C:484:GLY:HA2	1.73	0.70
1:B:177:TYR:CZ	1:B:185:GLY:HA3	2.26	0.70
1:B:486:CYS:SG	3:B:731:HOH:O	2.49	0.70
1:C:100:ARG:NH2	1:C:103:GLY:O	2.24	0.70
1:A:44:VAL:H	1:A:67:PRO:HA	1.56	0.70
1:C:303:THR:O	1:C:307:PHE:N	2.24	0.70
1:A:398:ARG:HD3	1:A:435:ARG:NH1	2.07	0.70
1:C:177:TYR:HD2	1:C:285:LEU:HD13	1.56	0.69
1:C:298:PRO:HD2	1:C:301:VAL:HG12	1.73	0.69
1:C:408:ARG:O	1:C:417:GLN:NE2	2.25	0.69
1:A:367:GLY:HA2	1:A:380:GLY:HA3	1.74	0.69
1:C:109:ASP:OD2	1:C:126:SER:OG	2.08	0.69
1:C:166:ARG:NH1	1:C:191:ALA:O	2.25	0.69
1:C:203:HIS:ND1	1:C:452:TRP:HZ3	1.91	0.69
1:A:77:ARG:O	1:A:81:GLU:HG2	1.93	0.69
1:A:386:GLU:O	1:A:389:THR:OG1	2.11	0.69
1:B:427:MET:HE3	1:B:489:TRP:CE3	2.28	0.68
1:C:169:THR:O	1:C:295:ARG:NH2	2.26	0.68
1:C:450:VAL:HG22	1:C:451:ASN:H	1.58	0.68
1:B:423:ALA:HB2	1:B:445:GLU:HG3	1.74	0.68
1:C:203:HIS:ND1	1:C:452:TRP:CZ3	2.61	0.68
1:A:394:TRP:HB2	1:A:398:ARG:CZ	2.23	0.68
1:C:17:ASN:C	1:C:20:ARG:HH12	2.02	0.68
1:C:88:ARG:CB	1:C:90:LYS:HE3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:PRO:HG2	2:C:601:BLR:H22	1.75	0.68
1:A:13:VAL:HG13	1:A:15:LEU:HD21	1.74	0.68
1:B:408:ARG:HA	1:B:422:VAL:HG11	1.75	0.68
1:A:464:GLN:HB2	1:A:466:GLY:H	1.59	0.67
1:C:89:LEU:HD22	1:C:112:ALA:HB3	1.75	0.67
1:A:177:TYR:CZ	1:A:185:GLY:HA3	2.30	0.67
1:C:187:VAL:O	1:C:201:GLY:HA2	1.93	0.67
1:B:37:VAL:HG12	1:B:120:ILE:HG12	1.76	0.67
1:C:429:PHE:O	1:C:501:ARG:CZ	2.41	0.67
1:B:50:GLU:OE2	1:B:236:ARG:NH1	2.28	0.67
1:C:308:LEU:HD12	3:C:732:HOH:O	1.95	0.67
1:A:142:ARG:HD2	1:B:307:PHE:HB2	1.76	0.66
1:C:316:LEU:O	1:C:320:GLU:N	2.28	0.66
1:C:430:SER:HA	1:C:501:ARG:HD2	1.76	0.66
1:A:393:GLU:O	1:A:394:TRP:CG	2.48	0.66
1:B:409:LEU:HD22	1:B:416:ALA:HB2	1.78	0.66
1:B:393:GLU:HA	1:B:396:GLY:H	1.60	0.66
1:C:202:LEU:HB2	1:C:451:ASN:HD22	1.60	0.66
1:A:346:VAL:HA	1:A:511:ARG:HE	1.61	0.66
1:C:231:GLN:OE1	1:C:231:GLN:N	2.27	0.65
1:C:37:VAL:HG21	1:C:47:HIS:ND1	2.12	0.65
1:C:464:GLN:HE22	1:C:468:ARG:HH12	1.43	0.65
1:C:184:ASN:OD1	1:C:206:ALA:N	2.29	0.65
1:C:335:HIS:NE2	1:C:499:GLU:OE2	2.29	0.65
1:C:408:ARG:NH2	1:C:484:GLY:HA3	2.11	0.65
1:B:89:LEU:HD11	1:B:112:ALA:HB3	1.77	0.65
1:B:426:LEU:HD21	1:B:428:ALA:HB2	1.79	0.65
1:C:486:CYS:SG	1:C:489:TRP:NE1	2.66	0.65
1:A:394:TRP:HB3	1:A:398:ARG:HG3	1.78	0.65
1:B:422:VAL:HG22	3:B:731:HOH:O	1.96	0.65
1:A:243:GLU:HG3	1:A:244:PRO:HD2	1.77	0.65
1:B:420:GLN:O	1:B:423:ALA:HB3	1.97	0.65
1:C:202:LEU:CD2	1:C:452:TRP:HA	2.20	0.65
1:C:509:LEU:HD12	1:C:510:GLN:NE2	2.12	0.65
2:C:601:BLR:NA	3:C:703:HOH:O	2.21	0.64
1:A:30:GLN:HE22	1:A:225:ILE:HA	1.62	0.64
1:B:425:GLY:N	1:B:443:ARG:H	1.82	0.64
1:B:423:ALA:O	1:B:444:PRO:HA	1.98	0.64
1:B:367:GLY:HA2	1:B:380:GLY:HA3	1.78	0.64
1:A:80:LEU:HD11	1:A:97:VAL:HG22	1.79	0.64
1:C:170:GLY:HA3	1:C:295:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HG	1:C:169:THR:H	1.63	0.63
1:B:147:ARG:NH2	1:B:163:GLN:OE1	2.18	0.63
1:B:243:GLU:OE2	1:B:243:GLU:N	2.25	0.63
1:C:36:LEU:HD13	1:C:45:LEU:HD21	1.79	0.63
1:A:411:ARG:NH2	1:A:412:GLU:OE1	2.32	0.63
1:B:44:VAL:HA	1:B:67:PRO:HA	1.79	0.63
1:C:88:ARG:HB3	1:C:90:LYS:CE	2.26	0.63
1:B:383:PRO:O	1:B:385:ASP:N	2.32	0.63
1:C:217:TYR:OH	2:C:601:BLR:H33	1.99	0.63
1:B:392:ILE:O	1:B:395:LEU:HB2	1.98	0.63
1:A:130:GLU:HG3	1:A:133:PRO:CG	2.29	0.63
1:B:340:GLU:O	1:B:344:ARG:HG3	1.99	0.63
1:B:423:ALA:HB2	1:B:445:GLU:CG	2.29	0.62
1:C:224:ILE:CG2	1:C:302:ARG:HD3	2.29	0.62
1:A:39:SER:HB3	1:A:44:VAL:HG13	1.81	0.62
1:C:316:LEU:HG	1:C:317:ALA:N	2.14	0.62
1:C:478:TRP:NE1	1:C:480:GLU:OE1	2.33	0.62
1:C:171:PHE:HB3	1:C:173:ARG:O	1.99	0.62
1:C:101:VAL:HG21	1:C:106:ARG:NH2	2.14	0.62
1:C:37:VAL:HG22	1:C:47:HIS:H	1.64	0.62
1:A:56:LEU:HD11	1:A:99:TRP:CZ2	2.34	0.62
1:B:212:GLN:OE1	1:B:212:GLN:N	2.30	0.62
1:A:394:TRP:HB2	1:A:398:ARG:NH1	2.14	0.62
1:C:396:GLY:HA3	1:C:398:ARG:HG3	1.81	0.62
1:C:162:VAL:HB	1:C:191:ALA:HB2	1.81	0.62
1:B:416:ALA:HA	1:B:419:PHE:CD2	2.34	0.61
1:A:69:GLY:C	1:A:77:ARG:HH11	2.07	0.61
1:C:487:LEU:HB2	1:C:489:TRP:HD1	1.65	0.61
1:A:15:LEU:HD22	1:A:19:ASP:OD2	2.00	0.61
1:A:400:GLY:O	1:A:401:GLU:HG3	2.00	0.61
1:C:312:MET:SD	1:C:313:SER:OG	2.53	0.61
1:C:320:GLU:N	1:C:321:GLY:HA3	2.15	0.61
1:A:142:ARG:NH2	1:B:306:GLU:CG	2.59	0.61
1:B:426:LEU:HA	1:B:441:TRP:O	2.01	0.61
1:C:278:LYS:CG	1:C:316:LEU:HD22	2.31	0.61
1:C:298:PRO:HB2	1:C:301:VAL:HG12	1.81	0.61
1:C:192:ARG:HD2	1:C:194:ALA:HA	1.83	0.61
1:C:492:TYR:O	1:C:496:ALA:HB2	2.01	0.61
1:B:173:ARG:NH2	1:B:197:ASP:O	2.34	0.60
1:C:93:ASN:HA	1:C:95:LEU:HD12	1.83	0.60
1:A:84:LEU:HD21	1:A:121:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ASP:HA	1:C:212:GLN:HG2	1.83	0.60
1:C:164:GLU:O	1:C:168:LEU:CD2	2.48	0.60
1:C:311:VAL:HG12	1:C:315:LEU:HD12	1.81	0.60
1:C:186:SER:HA	1:C:203:HIS:CD2	2.36	0.60
1:C:202:LEU:C	1:C:202:LEU:CD1	2.73	0.60
1:B:100:ARG:HH11	1:B:105:ASP:CG	2.08	0.60
1:B:406:THR:O	1:B:489:TRP:NE1	2.32	0.60
1:B:422:VAL:HG12	1:B:484:GLY:O	2.00	0.60
1:C:430:SER:HA	1:C:501:ARG:HD3	1.82	0.60
1:B:363:VAL:HG21	1:B:441:TRP:CG	2.36	0.60
1:B:330:ARG:O	1:B:334:ILE:N	2.25	0.60
1:B:478:TRP:CZ3	1:B:480:GLU:HB2	2.37	0.60
1:C:276:LEU:HG	1:C:312:MET:HE2	1.82	0.60
1:C:489:TRP:HB2	1:C:494:VAL:HG22	1.84	0.60
1:C:113:HIS:CE1	1:C:120:ILE:HD11	2.37	0.59
1:C:359:LEU:HD11	1:C:441:TRP:NE1	2.16	0.59
1:B:422:VAL:CG1	1:B:484:GLY:O	2.50	0.59
1:B:495:GLU:OE1	1:B:495:GLU:N	2.32	0.59
1:C:299:TYR:O	1:C:303:THR:OG1	2.10	0.59
1:B:326:ASP:CG	1:B:327:GLN:HA	2.28	0.59
1:B:363:VAL:HG21	1:B:441:TRP:CD1	2.38	0.59
1:C:364:HIS:CE1	1:C:490:LYS:HD2	2.38	0.59
1:B:328:ARG:CG	1:B:329:ILE:H	2.16	0.58
1:C:73:GLU:OE2	1:C:76:VAL:HG22	2.03	0.58
1:B:321:GLY:O	1:B:323:GLU:HG2	2.04	0.58
1:B:43:LEU:HD12	1:B:81:GLU:HG2	1.84	0.58
1:B:342:MET:HE1	1:B:504:ILE:HG12	1.85	0.58
1:C:259:HIS:CE1	2:C:601:BLR:H9	2.39	0.58
1:A:42:GLY:O	1:A:43:LEU:HD23	2.04	0.58
1:C:19:ASP:HB3	1:C:212:GLN:NE2	2.17	0.58
1:A:130:GLU:HG3	1:A:133:PRO:HG2	1.85	0.58
1:C:209:ILE:HG12	3:C:727:HOH:O	2.02	0.58
1:A:257:PRO:HA	1:A:260:LEU:HD12	1.86	0.58
1:B:483:ARG:O	1:B:485:ARG:N	2.36	0.58
1:A:17:ASN:HA	1:A:20:ARG:HH12	1.68	0.58
1:C:175:ILE:CD1	1:C:187:VAL:CG1	2.82	0.58
1:C:217:TYR:OH	2:C:601:BLR:H1	2.04	0.57
1:C:327:GLN:NE2	1:C:493:GLU:OE1	2.35	0.57
1:A:401:GLU:HG2	3:A:707:HOH:O	2.02	0.57
1:B:166:ARG:O	1:B:170:GLY:N	2.34	0.57
1:B:338:LEU:O	1:B:342:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:GLY:O	1:C:58:ASN:ND2	2.37	0.57
1:A:310:GLU:OE2	1:B:149:ARG:NH1	2.37	0.57
1:C:501:ARG:O	1:C:502:ARG:HD3	2.04	0.57
1:A:247:LEU:O	1:A:253:ARG:HD3	2.05	0.57
1:A:223:ARG:HH21	1:A:273:SER:HG	1.51	0.57
1:A:389:THR:HG22	1:A:413:TYR:HE2	1.68	0.57
1:B:384:SER:O	1:B:386:GLU:N	2.37	0.57
1:C:179:PHE:CE1	1:C:285:LEU:HD12	2.40	0.57
1:C:454:GLY:HA3	1:C:472:ARG:HD3	1.87	0.57
1:C:204:PHE:HB2	2:C:601:BLR:H16	1.86	0.57
1:C:338:LEU:HD23	1:C:504:ILE:HG12	1.86	0.57
1:A:16:THR:O	1:A:20:ARG:NH2	2.38	0.57
1:A:389:THR:HG22	1:A:413:TYR:CE2	2.40	0.57
1:C:124:GLU:OE2	1:C:302:ARG:NH2	2.37	0.57
1:B:13:VAL:HA	1:B:14:ASP:CB	2.31	0.56
1:C:89:LEU:O	1:C:91:GLN:N	2.38	0.56
1:C:278:LYS:HB3	1:C:316:LEU:CD2	2.35	0.56
1:B:460:VAL:CG1	1:B:469:LEU:HD22	2.34	0.56
1:C:95:LEU:HD12	1:C:95:LEU:H	1.69	0.56
1:C:178:ARG:NH2	1:C:179:PHE:HB2	2.21	0.56
1:C:408:ARG:HH21	1:C:421:GLU:CD	2.13	0.56
1:B:341:ARG:HG3	1:B:355:GLN:HE21	1.70	0.56
1:C:17:ASN:HA	1:C:20:ARG:HH12	1.71	0.56
1:A:88:ARG:NH2	1:B:150:ASP:O	2.39	0.56
1:A:429:PHE:CD1	1:A:501:ARG:HG3	2.41	0.56
1:B:419:PHE:C	1:B:421:GLU:H	2.13	0.56
1:C:173:ARG:NH2	1:C:199:TYR:CE1	2.73	0.56
1:C:175:ILE:CD1	1:C:187:VAL:HG13	2.29	0.56
1:C:276:LEU:O	1:C:283:TRP:N	2.37	0.56
1:A:388:LEU:O	1:A:392:ILE:HG22	2.06	0.56
1:A:452:TRP:CD2	1:A:456:PRO:HG3	2.41	0.56
1:C:297:VAL:CG2	1:C:301:VAL:CG1	2.81	0.56
1:A:152:ARG:HG3	1:A:156:GLU:CD	2.31	0.56
1:C:310:GLU:N	1:C:312:MET:HG3	2.20	0.56
1:A:359:LEU:HD23	1:A:379:LEU:HD12	1.86	0.56
1:C:152:ARG:O	1:C:322:ASN:HB3	2.06	0.56
1:B:120:ILE:HD11	1:B:245:LEU:HD11	1.88	0.55
1:C:100:ARG:NH1	1:C:105:ASP:CG	2.65	0.55
1:C:278:LYS:HD3	1:C:313:SER:HA	1.87	0.55
1:B:258:ILE:CD1	2:B:601:BLR:H24	2.37	0.55
1:C:202:LEU:HD21	1:C:452:TRP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PHE:O	1:C:310:GLU:HG3	2.07	0.55
1:C:318:ALA:O	1:C:319:LYS:HG3	2.06	0.55
1:A:455:ASN:OD1	1:A:457:THR:OG1	2.24	0.55
1:A:253:ARG:NH2	2:A:601:BLR:O2D	2.33	0.55
1:C:154:LEU:CD2	1:C:155:GLN:HE22	2.00	0.55
1:A:15:LEU:HB3	1:A:19:ASP:OD2	2.07	0.55
1:A:19:ASP:C	1:A:20:ARG:HD2	2.32	0.55
1:C:152:ARG:C	1:C:319:LYS:HG2	2.31	0.55
1:C:451:ASN:CA	1:C:480:GLU:HG2	2.37	0.55
1:C:129:ARG:HD3	1:C:298:PRO:HG3	1.89	0.55
1:B:374:GLY:CA	1:B:375:ARG:HB2	2.36	0.55
1:A:371:HIS:ND1	1:A:376:THR:HG22	2.22	0.55
1:B:44:VAL:HG22	1:B:67:PRO:HB3	1.90	0.55
1:C:243:GLU:CD	1:C:243:GLU:H	2.15	0.54
1:C:122:GLU:OE1	1:C:251:VAL:N	2.39	0.54
1:B:330:ARG:HA	1:B:333:SER:HB3	1.89	0.54
1:B:337:ALA:O	1:B:341:ARG:HG2	2.07	0.54
1:C:372:PHE:CE2	1:C:437:ASN:HB2	2.43	0.54
1:C:381:GLN:HG2	1:C:382:ALA:H	1.72	0.54
1:C:429:PHE:HB3	1:C:498:SER:HB3	1.88	0.54
1:C:429:PHE:CA	1:C:501:ARG:NH1	2.69	0.54
1:C:120:ILE:O	1:C:120:ILE:HD12	2.08	0.54
1:C:144:GLY:HA3	1:C:308:LEU:HD11	1.89	0.54
1:C:198:PRO:HG2	1:C:200:LEU:CD1	2.38	0.54
1:C:451:ASN:N	1:C:480:GLU:HG2	2.23	0.54
1:B:324:ASP:CG	1:B:328:ARG:NH2	2.66	0.54
1:A:183:TRP:CD1	1:A:214:ARG:HH21	2.26	0.54
1:C:173:ARG:NH2	1:C:199:TYR:CZ	2.70	0.54
1:C:178:ARG:NH2	1:C:283:TRP:O	2.39	0.54
1:A:16:THR:OG1	1:A:17:ASN:N	2.33	0.54
1:A:142:ARG:CD	1:B:307:PHE:HB2	2.38	0.54
1:B:328:ARG:CG	1:B:329:ILE:N	2.71	0.54
1:C:179:PHE:HD1	1:C:284:GLY:HA2	1.72	0.54
1:C:187:VAL:HB	1:C:202:LEU:N	2.19	0.54
1:C:456:PRO:HD2	1:C:478:TRP:CZ2	2.41	0.54
1:A:80:LEU:HD13	3:A:718:HOH:O	2.08	0.54
1:A:81:GLU:O	1:A:85:ARG:HD2	2.08	0.54
1:A:142:ARG:HH11	1:B:307:PHE:HA	1.34	0.54
1:B:407:ASP:O	1:B:485:ARG:HA	2.08	0.54
1:B:413:TYR:CE2	1:B:415:GLU:HB2	2.43	0.53
1:C:505:ILE:HG12	1:C:506:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:C	1:B:435:ARG:N	2.66	0.53
1:C:487:LEU:H	1:C:487:LEU:HD12	1.73	0.53
1:A:142:ARG:HH12	1:B:306:GLU:C	2.15	0.53
1:C:158:CYS:SG	1:C:176:ILE:HD13	2.48	0.53
1:C:277:MET:O	1:C:278:LYS:HD3	2.09	0.53
1:C:451:ASN:HA	1:C:480:GLU:HG2	1.90	0.53
1:B:500:LEU:O	1:B:504:ILE:HG13	2.09	0.53
1:C:101:VAL:HG21	1:C:106:ARG:CZ	2.39	0.53
1:C:162:VAL:HA	1:C:165:VAL:HG22	1.90	0.53
1:C:171:PHE:CD1	1:C:288:CYS:HB3	2.43	0.53
1:C:429:PHE:CA	1:C:501:ARG:HH12	2.22	0.53
1:C:275:SER:HA	1:C:285:LEU:HA	1.91	0.53
1:A:30:GLN:HG2	1:A:230:TYR:CZ	2.44	0.53
1:B:32:HIS:CE1	1:B:226:PRO:HG2	2.44	0.53
1:A:385:ASP:C	1:A:387:ALA:H	2.16	0.53
1:B:60:ALA:O	1:B:64:LEU:HD12	2.09	0.53
1:C:432:SER:O	1:C:434:GLY:N	2.38	0.53
1:C:487:LEU:HB2	1:C:489:TRP:CD1	2.43	0.53
1:A:394:TRP:HB3	1:A:398:ARG:CG	2.37	0.53
1:C:278:LYS:HG2	1:C:283:TRP:CB	2.37	0.53
1:A:42:GLY:HA3	1:A:85:ARG:NH2	2.20	0.52
1:B:460:VAL:HG11	1:B:469:LEU:HD22	1.92	0.52
1:C:148:LEU:HD11	1:C:161:VAL:HG11	1.91	0.52
1:C:178:ARG:HD2	1:C:179:PHE:H	1.73	0.52
1:C:471:PRO:CG	2:C:601:BLR:H22	2.40	0.52
1:B:45:LEU:HD22	1:B:63:LEU:HB3	1.91	0.52
1:C:185:GLY:C	1:C:203:HIS:CD2	2.87	0.52
1:C:202:LEU:CB	1:C:451:ASN:ND2	2.71	0.52
1:C:88:ARG:NH2	1:C:90:LYS:HD3	2.25	0.52
1:C:162:VAL:O	1:C:165:VAL:HG22	2.09	0.52
1:A:131:ALA:HA	1:B:134:PHE:CE1	2.44	0.52
1:C:183:TRP:HE3	1:C:214:ARG:HH21	1.57	0.52
1:A:214:ARG:HB3	1:A:282:LEU:HD23	1.91	0.52
1:C:78:GLU:HG3	3:C:709:HOH:O	2.09	0.52
1:C:111:ILE:HD12	1:C:299:TYR:CZ	2.45	0.52
1:C:261:GLU:O	1:C:264:HIS:HB3	2.09	0.52
1:B:274:ILE:HB	1:B:286:ILE:HB	1.91	0.52
1:B:501:ARG:O	1:B:505:ILE:HG13	2.10	0.52
1:C:138:PHE:N	3:C:710:HOH:O	2.42	0.52
1:C:214:ARG:HA	1:C:217:TYR:CD2	2.39	0.52
1:C:509:LEU:HD12	1:C:509:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLN:HA	1:C:158:CYS:HB2	1.92	0.52
1:C:140:ALA:O	1:C:144:GLY:N	2.41	0.51
1:B:114:ARG:HA	1:B:118:ARG:O	2.10	0.51
1:C:124:GLU:CD	1:C:302:ARG:HH22	2.18	0.51
1:C:319:LYS:HA	1:C:322:ASN:HB2	1.93	0.51
1:C:349:VAL:HG12	1:C:375:ARG:NH1	2.25	0.51
1:C:440:LEU:HD22	1:C:441:TRP:H	1.76	0.51
1:B:409:LEU:H	1:B:422:VAL:HB	1.74	0.51
1:C:175:ILE:HD11	1:C:187:VAL:C	2.35	0.51
1:A:464:GLN:N	1:A:465:GLY:HA2	2.26	0.51
1:C:217:TYR:CD1	1:C:223:ARG:NH1	2.78	0.51
1:C:503:SER:C	1:C:505:ILE:H	2.18	0.51
1:B:48:ALA:O	1:B:236:ARG:N	2.43	0.51
1:C:329:ILE:HD13	1:C:332:LYS:HZ3	1.75	0.51
1:A:160:ALA:O	1:A:164:GLU:HG2	2.11	0.51
1:C:73:GLU:CD	1:C:76:VAL:H	2.19	0.51
1:C:370:ILE:HD11	1:C:375:ARG:HH11	1.75	0.51
1:A:32:HIS:NE2	1:A:226:PRO:HG2	2.26	0.51
1:C:175:ILE:HD11	1:C:188:ILE:N	2.26	0.51
1:A:78:GLU:OE2	1:A:81:GLU:HG3	2.11	0.51
1:C:495:GLU:C	1:C:497:ALA:H	2.18	0.51
1:C:447:VAL:HG22	1:C:482:VAL:HG13	1.94	0.51
1:A:142:ARG:HD2	1:B:307:PHE:CD1	2.47	0.50
1:B:409:LEU:CD2	1:B:413:TYR:HB3	2.40	0.50
1:B:486:CYS:SG	1:B:487:LEU:N	2.83	0.50
1:B:327:GLN:O	1:B:328:ARG:C	2.54	0.50
1:C:143:ASP:OD1	1:C:146:SER:HB2	2.10	0.50
1:C:328:ARG:O	1:C:332:LYS:NZ	2.45	0.50
1:C:360:LEU:HD13	1:C:366:HIS:CE1	2.47	0.50
1:A:208:ASP:OD2	1:A:472:ARG:NH1	2.44	0.50
1:C:278:LYS:NZ	1:C:316:LEU:HB3	2.26	0.50
1:C:307:PHE:O	1:C:309:GLY:N	2.44	0.50
1:A:78:GLU:N	1:A:79:PRO:HD2	2.26	0.50
1:B:431:MET:HB2	1:B:437:ASN:HB2	1.94	0.50
1:C:17:ASN:CA	1:C:20:ARG:HH12	2.24	0.50
1:C:459:ALA:C	1:C:471:PRO:HB3	2.36	0.50
1:C:509:LEU:CD1	1:C:510:GLN:NE2	2.74	0.50
1:C:192:ARG:HG3	1:C:198:PRO:HB3	1.93	0.50
1:C:270:ALA:HB3	1:C:290:GLN:HB3	1.93	0.50
1:C:278:LYS:HB3	1:C:316:LEU:HD21	1.93	0.50
1:B:177:TYR:OH	1:B:204:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:C	1:B:421:GLU:N	2.68	0.50
1:C:37:VAL:HG22	1:C:47:HIS:N	2.27	0.50
1:C:224:ILE:HG21	1:C:302:ARG:HD3	1.93	0.50
1:C:314:SER:N	1:C:316:LEU:HD23	2.27	0.50
1:B:366:HIS:HB2	1:B:444:PRO:HD3	1.94	0.50
1:C:120:ILE:HD12	1:C:120:ILE:C	2.36	0.50
1:C:220:ASN:OD1	1:C:221:TRP:N	2.42	0.50
1:C:429:PHE:C	1:C:501:ARG:HH12	2.10	0.50
1:C:202:LEU:O	1:C:202:LEU:CD1	2.58	0.50
1:C:408:ARG:NH2	1:C:421:GLU:CD	2.69	0.50
1:C:157:LEU:O	1:C:161:VAL:HG22	2.12	0.49
1:A:378:VAL:C	1:A:379:LEU:HD23	2.37	0.49
1:A:395:LEU:HA	1:A:398:ARG:HD2	1.94	0.49
1:A:461:GLU:HB3	1:A:470:HIS:O	2.13	0.49
1:C:115:HIS:CD2	1:C:116:GLN:HG2	2.47	0.49
1:C:137:PHE:HB3	3:C:710:HOH:O	2.11	0.49
1:C:342:MET:HG2	1:C:504:ILE:HG23	1.94	0.49
1:C:492:TYR:O	1:C:493:GLU:HG3	2.12	0.49
1:A:337:ALA:O	1:A:340:GLU:HG2	2.11	0.49
1:C:202:LEU:HD21	1:C:451:ASN:C	2.38	0.49
1:C:328:ARG:HG3	1:C:332:LYS:HZ2	1.77	0.49
1:C:335:HIS:HA	3:C:726:HOH:O	2.12	0.49
1:A:370:ILE:O	1:A:376:THR:HA	2.13	0.49
1:B:15:LEU:HD13	1:B:19:ASP:HB3	1.95	0.49
1:B:406:THR:C	1:B:489:TRP:HE1	2.19	0.49
1:C:421:GLU:HG3	1:C:422:VAL:N	2.27	0.49
1:C:486:CYS:HG	1:C:489:TRP:NE1	2.10	0.49
1:A:44:VAL:N	1:A:67:PRO:HA	2.26	0.49
1:A:395:LEU:CA	1:A:398:ARG:HD2	2.43	0.49
1:C:450:VAL:HG22	1:C:451:ASN:N	2.28	0.49
1:C:359:LEU:HD12	1:C:359:LEU:O	2.13	0.48
1:C:447:VAL:HG23	1:C:482:VAL:HG22	1.94	0.48
1:A:19:ASP:OD1	1:A:210:PRO:HB3	2.13	0.48
1:B:63:LEU:HD23	1:B:71:PHE:CZ	2.48	0.48
1:C:202:LEU:CD2	1:C:451:ASN:ND2	2.66	0.48
1:C:76:VAL:C	1:C:79:PRO:HD2	2.38	0.48
1:C:134:PHE:HB2	1:C:135:LEU:HD22	1.96	0.48
1:C:276:LEU:HG	1:C:312:MET:CE	2.44	0.48
1:C:315:LEU:HD13	3:C:706:HOH:O	2.13	0.48
1:C:489:TRP:CE3	1:C:494:VAL:HG13	2.49	0.48
1:B:425:GLY:O	1:B:442:PHE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:NH1	1:B:483:ARG:HB2	2.29	0.48
1:C:19:ASP:C	1:C:20:ARG:HD3	2.38	0.48
1:C:285:LEU:HD21	3:C:727:HOH:O	2.13	0.48
1:C:440:LEU:CD2	1:C:441:TRP:H	2.26	0.48
1:C:489:TRP:HE3	1:C:494:VAL:HG22	1.77	0.48
1:B:433:ARG:C	1:B:435:ARG:H	2.19	0.48
1:C:217:TYR:HD1	1:C:223:ARG:NH1	2.12	0.48
1:C:238:LEU:O	1:C:241:HIS:HB2	2.14	0.48
1:C:72:ILE:O	1:C:72:ILE:HG13	2.13	0.48
1:A:44:VAL:HA	1:A:67:PRO:HA	1.96	0.48
1:B:325:TYR:CG	1:B:325:TYR:O	2.65	0.48
1:B:450:VAL:HG13	1:B:452:TRP:HE1	1.78	0.48
1:C:350:SER:OG	1:C:375:ARG:NH2	2.47	0.48
1:B:463:ASP:HB3	1:B:466:GLY:HA3	1.96	0.48
1:A:210:PRO:HB2	1:A:212:GLN:OE1	2.13	0.48
1:A:258:ILE:HG13	1:A:471:PRO:HD3	1.96	0.48
1:B:378:VAL:HG12	1:B:379:LEU:H	1.78	0.47
1:C:37:VAL:HG13	1:C:47:HIS:HB2	1.95	0.47
1:B:378:VAL:HG12	1:B:379:LEU:N	2.29	0.47
1:C:113:HIS:HE1	3:C:723:HOH:O	1.96	0.47
1:A:300:GLU:OE2	1:B:142:ARG:NH2	2.47	0.47
1:C:176:ILE:HD12	1:C:176:ILE:H	1.80	0.47
1:B:258:ILE:HG13	1:B:259:HIS:N	2.28	0.47
1:C:162:VAL:CB	1:C:191:ALA:HB2	2.44	0.47
1:C:359:LEU:HB2	1:C:362:LEU:HD11	1.95	0.47
1:C:361:GLU:O	3:C:702:HOH:O	2.20	0.47
1:A:177:TYR:OH	1:A:185:GLY:HA3	2.15	0.47
1:A:327:GLN:HB3	1:A:492:TYR:CZ	2.50	0.47
1:C:116:GLN:NE2	3:C:704:HOH:O	2.24	0.47
1:C:411:ARG:HA	1:C:411:ARG:CZ	2.45	0.47
1:A:431:MET:HE2	1:A:439:VAL:HG23	1.95	0.47
1:A:44:VAL:HA	1:A:66:ALA:O	2.14	0.47
1:A:236:ARG:HD2	1:A:236:ARG:HA	1.48	0.47
1:A:436:ASN:N	3:A:708:HOH:O	2.47	0.47
1:B:455:ASN:OD1	1:B:457:THR:HG23	2.14	0.47
1:B:457:THR:OG1	1:B:458:LYS:N	2.48	0.47
1:C:169:THR:HB	1:C:171:PHE:CD2	2.50	0.47
1:C:179:PHE:HA	1:C:185:GLY:HA3	1.96	0.47
1:A:173:ARG:O	1:A:288:CYS:HA	2.14	0.47
1:B:434:GLY:C	1:B:435:ARG:HG3	2.40	0.47
1:B:507:VAL:O	1:B:511:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:HIS:HE1	2:C:601:BLR:H9	1.80	0.47
1:C:318:ALA:O	1:C:322:ASN:HB2	2.14	0.47
1:A:20:ARG:CD	1:A:20:ARG:N	2.78	0.47
1:B:409:LEU:HD23	1:B:413:TYR:HB3	1.95	0.47
1:B:445:GLU:CD	1:B:483:ARG:HG3	2.40	0.47
1:C:221:TRP:NE1	1:C:277:MET:HE3	2.29	0.47
1:C:307:PHE:CD2	1:C:310:GLU:HG2	2.49	0.47
1:C:328:ARG:HG3	1:C:332:LYS:NZ	2.30	0.47
1:C:19:ASP:HB3	1:C:212:GLN:HE21	1.79	0.46
1:C:115:HIS:NE2	1:C:246:ASP:OD2	2.48	0.46
1:C:193:ASP:CG	1:C:195:ARG:HH21	2.23	0.46
1:C:258:ILE:HD11	2:C:601:BLR:H27	1.97	0.46
1:A:192:ARG:HH21	1:C:81:GLU:CD	2.22	0.46
1:A:208:ASP:HA	2:A:601:BLR:C1C	2.45	0.46
1:C:69:GLY:HA2	1:C:72:ILE:HG12	1.97	0.46
1:C:144:GLY:HA3	1:C:308:LEU:CD1	2.44	0.46
1:C:151:ALA:HB3	1:C:157:LEU:HD13	1.91	0.46
1:C:170:GLY:CA	1:C:295:ARG:HH21	2.26	0.46
1:C:328:ARG:O	1:C:332:LYS:HG3	2.14	0.46
1:B:426:LEU:HD23	1:B:427:MET:N	2.30	0.46
1:C:73:GLU:HB3	1:C:100:ARG:CG	2.31	0.46
1:A:388:LEU:HD12	1:A:388:LEU:H	1.80	0.46
1:C:110:GLY:HA2	1:C:122:GLU:O	2.15	0.46
1:A:399:THR:O	1:A:401:GLU:N	2.48	0.46
1:B:24:HIS:HD2	3:B:717:HOH:O	1.99	0.46
1:B:126:SER:C	1:B:129:ARG:HG3	2.40	0.46
1:C:37:VAL:CG2	1:C:47:HIS:ND1	2.78	0.46
1:C:169:THR:OG1	1:C:170:GLY:N	2.48	0.46
1:C:192:ARG:NH1	1:C:198:PRO:HG3	2.30	0.46
1:A:366:HIS:HB3	3:A:741:HOH:O	2.14	0.46
1:A:395:LEU:HG	1:A:396:GLY:H	1.80	0.46
1:C:21:GLU:OE1	1:C:23:ILE:HG22	2.15	0.46
1:A:22:PRO:HA	3:A:740:HOH:O	2.14	0.46
1:B:49:SER:HA	1:B:235:VAL:HA	1.97	0.46
1:C:168:LEU:HD11	1:C:305:CYS:HG	1.74	0.46
1:A:175:ILE:HD11	1:A:287:SER:HB3	1.98	0.46
1:A:365:ALA:HB1	1:A:442:PHE:O	2.15	0.46
1:C:141:VAL:HG13	3:C:701:HOH:O	2.15	0.46
1:B:187:VAL:CG2	2:B:601:BLR:H19	2.46	0.46
1:C:173:ARG:HE	1:C:173:ARG:HB2	1.49	0.46
1:A:342:MET:SD	1:A:352:LEU:HD21	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:HA	3:C:730:HOH:O	2.15	0.45
1:C:394:TRP:HZ2	1:C:426:LEU:HD21	1.82	0.45
1:A:40:GLU:HA	1:A:42:GLY:N	2.32	0.45
1:A:458:LYS:O	1:A:460:VAL:N	2.45	0.45
1:C:273:SER:HA	1:C:286:ILE:O	2.16	0.45
1:B:13:VAL:CA	1:B:14:ASP:HB2	2.34	0.45
1:B:503:SER:O	1:B:507:VAL:HG22	2.16	0.45
1:C:108:PHE:HA	1:C:125:PRO:HA	1.99	0.45
1:C:299:TYR:O	1:C:303:THR:N	2.36	0.45
1:C:307:PHE:O	1:C:309:GLY:C	2.59	0.45
1:C:316:LEU:HD12	1:C:316:LEU:C	2.41	0.45
1:C:360:LEU:HD13	1:C:366:HIS:HE1	1.80	0.45
1:A:275:SER:O	1:A:276:LEU:HD23	2.16	0.45
1:C:17:ASN:HA	1:C:20:ARG:NH1	2.31	0.45
1:B:324:ASP:O	1:B:326:ASP:C	2.59	0.45
1:B:377:THR:O	1:B:377:THR:OG1	2.35	0.45
1:B:458:LYS:NZ	1:B:461:GLU:OE1	2.41	0.45
1:C:140:ALA:HB3	3:C:701:HOH:O	2.15	0.45
1:C:164:GLU:O	1:C:166:ARG:N	2.49	0.45
1:A:299:TYR:CZ	1:A:303:THR:HG21	2.52	0.45
1:B:365:ALA:HB1	1:B:442:PHE:O	2.16	0.45
1:B:421:GLU:O	1:B:424:ALA:N	2.34	0.45
1:C:89:LEU:HD13	1:C:113:HIS:HA	1.98	0.45
1:C:171:PHE:CZ	1:C:272:MET:HB2	2.52	0.45
1:C:310:GLU:HA	1:C:312:MET:HE3	1.99	0.45
2:C:601:BLR:NB	2:C:601:BLR:H4	2.32	0.45
1:B:425:GLY:O	1:B:489:TRP:HH2	2.00	0.45
1:A:428:ALA:HA	1:A:439:VAL:O	2.17	0.45
1:B:328:ARG:HG2	1:B:329:ILE:H	1.81	0.45
1:C:479:LYS:H	1:C:479:LYS:HG3	1.58	0.45
1:A:147:ARG:HG2	1:A:160:ALA:HB1	1.99	0.45
1:A:197:ASP:OD2	1:C:77:ARG:NH1	2.50	0.45
1:C:209:ILE:HD11	2:C:601:BLR:H14	1.97	0.45
1:B:502:ARG:HA	1:B:502:ARG:HD3	1.70	0.45
1:C:202:LEU:HA	1:C:202:LEU:HD22	1.62	0.45
1:C:274:ILE:HG23	1:C:274:ILE:O	2.17	0.45
1:C:429:PHE:H	1:C:497:ALA:HB3	1.81	0.45
1:A:89:LEU:HD12	1:A:113:HIS:HA	1.99	0.44
1:A:395:LEU:N	1:A:398:ARG:HD2	2.33	0.44
1:B:69:GLY:O	1:B:77:ARG:HD3	2.16	0.44
1:C:98:VAL:HG23	3:C:719:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:HG3	2:C:601:BLR:CAC	2.42	0.44
1:C:310:GLU:CA	1:C:312:MET:HG3	2.47	0.44
1:C:432:SER:C	1:C:434:GLY:H	2.25	0.44
1:B:28:ALA:HB1	1:B:232:PRO:HB3	1.98	0.44
1:C:55:VAL:HG12	1:C:108:PHE:CE2	2.52	0.44
1:C:135:LEU:HA	1:C:138:PHE:HB3	1.99	0.44
1:C:179:PHE:CD1	1:C:284:GLY:HA2	2.51	0.44
1:A:289:HIS:CE1	2:A:601:BLR:OB	2.71	0.44
1:C:113:HIS:CD2	1:C:120:ILE:CD1	2.95	0.44
1:C:406:THR:HG23	1:C:409:LEU:HG	1.99	0.44
1:A:19:ASP:OD1	1:A:19:ASP:N	2.49	0.44
1:B:466:GLY:HA2	1:B:467:PRO:HD3	1.87	0.44
1:C:286:ILE:HG22	1:C:288:CYS:SG	2.57	0.44
1:B:34:VAL:HG11	1:B:56:LEU:HD11	1.99	0.44
1:B:384:SER:HB2	1:B:388:LEU:HB2	1.98	0.44
1:B:502:ARG:HD2	3:B:725:HOH:O	2.17	0.44
1:C:133:PRO:HD2	1:C:136:SER:HB2	2.00	0.44
1:B:202:LEU:HD13	1:B:453:SER:HB2	1.99	0.44
1:C:311:VAL:O	1:C:314:SER:OG	2.35	0.44
1:B:349:VAL:HG21	1:B:372:PHE:CG	2.52	0.44
1:B:58:ASN:ND2	1:B:62:GLN:OE1	2.49	0.44
1:C:89:LEU:HD22	1:C:112:ALA:CB	2.47	0.44
1:A:463:ASP:HB2	1:A:468:ARG:HB2	2.00	0.43
1:B:483:ARG:HG2	1:B:484:GLY:N	2.32	0.43
1:C:100:ARG:NH2	1:C:104:VAL:C	2.76	0.43
1:C:169:THR:HB	1:C:171:PHE:HD2	1.83	0.43
1:C:420:GLN:O	1:C:421:GLU:HG2	2.18	0.43
1:A:129:ARG:HG3	1:B:138:PHE:CE1	2.53	0.43
2:B:601:BLR:OB	2:B:601:BLR:H18	2.17	0.43
1:C:168:LEU:HG	1:C:169:THR:N	2.31	0.43
1:C:238:LEU:HD23	1:C:239:PRO:HD2	2.00	0.43
1:C:297:VAL:O	1:C:297:VAL:HG13	2.18	0.43
1:A:175:ILE:HD12	1:A:175:ILE:C	2.43	0.43
1:A:183:TRP:CG	1:A:214:ARG:HH21	2.36	0.43
1:B:90:LYS:HE2	1:B:113:HIS:HA	2.00	0.43
1:B:431:MET:HG2	1:B:504:ILE:HG21	2.00	0.43
1:C:362:LEU:HD12	1:C:363:VAL:N	2.34	0.43
1:A:13:VAL:HG22	1:A:15:LEU:HD23	1.99	0.43
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.77	0.43
1:B:72:ILE:HG23	1:B:98:VAL:O	2.18	0.43
1:B:405:CYS:SG	1:B:427:MET:HE2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:C	1:C:166:ARG:N	2.74	0.43
1:C:221:TRP:HB3	1:C:275:SER:O	2.18	0.43
1:C:297:VAL:HA	1:C:298:PRO:HD3	1.51	0.43
1:C:340:GLU:HA	1:C:344:ARG:HB2	1.99	0.43
1:C:72:ILE:CD1	1:C:80:LEU:HD23	2.48	0.43
1:C:166:ARG:HA	1:C:169:THR:OG1	2.19	0.43
1:C:408:ARG:NH2	1:C:445:GLU:OE1	2.51	0.43
1:A:507:VAL:O	1:A:511:ARG:HG2	2.18	0.43
1:B:173:ARG:NH2	1:B:196:ALA:HB1	2.34	0.43
1:C:312:MET:C	1:C:314:SER:N	2.76	0.43
1:C:341:ARG:HA	1:C:345:GLU:CD	2.44	0.43
1:C:365:ALA:HA	1:C:443:ARG:HD3	2.01	0.43
1:C:470:HIS:ND1	1:C:471:PRO:HD2	2.34	0.43
1:C:497:ALA:HB1	1:C:501:ARG:CZ	2.45	0.43
1:C:278:LYS:HB3	1:C:316:LEU:HD22	1.99	0.43
1:A:262:TYR:CE2	1:A:266:MET:HE2	2.53	0.43
1:A:416:ALA:HA	1:A:419:PHE:CZ	2.54	0.43
1:B:217:TYR:N	1:B:217:TYR:CD1	2.85	0.43
1:C:36:LEU:HD13	1:C:45:LEU:CD2	2.46	0.43
1:A:29:ILE:HB	1:A:252:LEU:HB3	1.99	0.43
1:A:78:GLU:OE1	3:A:701:HOH:O	2.21	0.43
1:A:173:ARG:NH2	1:A:197:ASP:O	2.51	0.43
1:B:483:ARG:O	1:B:484:GLY:C	2.62	0.43
1:C:175:ILE:HD11	1:C:187:VAL:CA	2.49	0.43
1:C:262:TYR:HB2	1:C:470:HIS:CE1	2.54	0.43
1:B:242:GLY:N	1:B:243:GLU:OE2	2.52	0.43
1:C:192:ARG:CD	1:C:198:PRO:HB3	2.48	0.43
1:C:463:ASP:O	1:C:465:GLY:N	2.52	0.43
1:A:101:VAL:HG11	1:A:106:ARG:CZ	2.49	0.42
1:A:385:ASP:C	1:A:387:ALA:N	2.77	0.42
1:B:175:ILE:HD13	1:B:187:VAL:HG22	2.01	0.42
1:B:273:SER:HA	1:B:286:ILE:O	2.19	0.42
1:B:451:ASN:HB3	1:B:477:LEU:CD1	2.49	0.42
1:C:503:SER:C	1:C:505:ILE:N	2.75	0.42
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.83	0.42
1:B:223:ARG:NH1	1:B:275:SER:OG	2.48	0.42
1:C:30:GLN:HA	1:C:31:PRO:HD3	1.80	0.42
1:C:490:LYS:HG3	1:C:493:GLU:OE2	2.20	0.42
1:A:30:GLN:HG3	3:A:705:HOH:O	2.20	0.42
1:B:81:GLU:O	1:B:85:ARG:HG3	2.19	0.42
1:C:335:HIS:O	1:C:503:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ILE:O	1:C:507:VAL:HG22	2.20	0.42
1:A:179:PHE:CE2	1:A:282:LEU:HG	2.54	0.42
1:B:180:ASP:OD2	1:B:184:ASN:HB2	2.20	0.42
1:B:495:GLU:H	1:B:495:GLU:CD	2.19	0.42
1:A:394:TRP:HB2	1:A:398:ARG:NE	2.34	0.42
1:B:328:ARG:HG3	1:B:329:ILE:N	2.34	0.42
1:C:21:GLU:HA	1:C:22:PRO:HD3	1.87	0.42
1:A:209:ILE:O	1:A:214:ARG:NH1	2.36	0.42
1:C:82:ALA:O	1:C:86:SER:OG	2.37	0.42
1:C:221:TRP:N	1:C:221:TRP:CD1	2.86	0.42
1:A:169:THR:HG21	1:A:272:MET:HE1	2.01	0.42
1:B:73:GLU:HA	1:B:74:PRO:HD3	1.91	0.42
1:B:175:ILE:HB	1:B:187:VAL:HG13	2.02	0.42
1:B:460:VAL:HG12	1:B:469:LEU:HD22	2.00	0.42
1:B:511:ARG:O	1:B:514:GLU:HB2	2.19	0.42
1:C:309:GLY:O	1:C:312:MET:HE3	2.20	0.42
1:A:61:GLU:H	1:A:61:GLU:CD	2.26	0.42
1:A:334:ILE:HD11	1:A:361:GLU:OE1	2.20	0.42
1:B:476:GLU:OE1	1:B:476:GLU:N	2.53	0.42
1:C:73:GLU:O	1:C:77:ARG:NE	2.53	0.42
1:C:255:VAL:CG1	1:C:260:LEU:HD11	2.50	0.42
1:C:315:LEU:O	1:C:319:LYS:N	2.53	0.42
1:A:340:GLU:HG3	1:A:341:ARG:N	2.35	0.42
1:C:147:ARG:NH2	1:C:160:ALA:HA	2.34	0.42
1:C:178:ARG:O	1:C:185:GLY:HA3	2.19	0.42
1:C:295:ARG:HA	1:C:295:ARG:HH11	1.84	0.42
1:C:453:SER:C	1:C:478:TRP:HZ3	2.27	0.42
1:B:98:VAL:HA	1:B:106:ARG:O	2.19	0.41
1:C:174:ALA:HA	1:C:288:CYS:SG	2.60	0.41
1:C:180:ASP:N	1:C:180:ASP:OD1	2.51	0.41
1:B:140:ALA:O	1:B:144:GLY:HA3	2.20	0.41
1:B:360:LEU:HD23	1:B:360:LEU:HA	1.93	0.41
1:C:202:LEU:HD13	1:C:203:HIS:O	2.20	0.41
1:C:445:GLU:HG3	1:C:446:ALA:N	2.36	0.41
1:A:451:ASN:OD1	1:A:479:LYS:HE2	2.20	0.41
1:C:276:LEU:HD21	1:C:278:LYS:HE2	2.01	0.41
1:C:505:ILE:HG12	1:C:506:ASP:N	2.35	0.41
1:B:175:ILE:CD1	1:B:177:TYR:HB2	2.51	0.41
1:C:55:VAL:HG12	1:C:108:PHE:HE2	1.84	0.41
1:C:436:ASN:HA	1:C:437:ASN:HA	1.85	0.41
1:A:447:VAL:O	1:A:482:VAL:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.82	0.41
1:B:407:ASP:O	1:B:422:VAL:HG11	2.21	0.41
1:B:410:ALA:O	1:B:414:PRO:HG3	2.19	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.91	0.41
1:B:59:SER:H	1:B:62:GLN:NE2	2.18	0.41
1:C:221:TRP:CD1	1:C:277:MET:HE3	2.55	0.41
1:C:328:ARG:C	1:C:332:LYS:HZ2	2.29	0.41
1:C:439:VAL:HG13	1:C:500:LEU:HD23	2.01	0.41
1:A:30:GLN:OE1	1:A:226:PRO:HD2	2.21	0.41
1:C:178:ARG:CD	1:C:179:PHE:H	2.33	0.41
1:C:228:ILE:HG23	1:C:269:GLN:O	2.21	0.41
1:C:470:HIS:ND1	1:C:471:PRO:N	2.69	0.41
1:A:56:LEU:HD13	1:A:56:LEU:O	2.20	0.41
1:A:166:ARG:NH1	1:A:171:PHE:O	2.54	0.41
1:A:177:TYR:CE1	1:A:185:GLY:HA3	2.56	0.41
1:A:266:MET:HG3	1:A:475:PHE:CD2	2.56	0.41
1:A:366:HIS:O	1:A:380:GLY:HA3	2.21	0.41
1:A:394:TRP:CB	1:A:398:ARG:HG3	2.48	0.41
1:A:412:GLU:O	1:A:414:PRO:HD3	2.20	0.41
1:B:366:HIS:N	1:B:442:PHE:O	2.54	0.41
1:B:430:SER:CB	1:B:433:ARG:HH12	2.16	0.41
1:C:78:GLU:HB2	1:C:79:PRO:HD3	2.03	0.41
1:C:147:ARG:HH21	1:C:160:ALA:HA	1.86	0.41
1:C:199:TYR:O	1:C:200:LEU:C	2.64	0.41
1:C:391:LEU:O	1:C:392:ILE:HB	2.21	0.41
1:A:221:TRP:O	1:A:274:ILE:HA	2.22	0.41
1:B:464:GLN:HB2	1:B:465:GLY:C	2.46	0.41
1:C:88:ARG:HD2	1:C:88:ARG:HA	1.89	0.41
1:C:97:VAL:CG2	1:C:110:GLY:H	2.34	0.41
1:C:168:LEU:HD23	1:C:168:LEU:H	1.86	0.41
1:C:454:GLY:HA3	1:C:472:ARG:HH21	1.85	0.41
1:C:495:GLU:C	1:C:497:ALA:N	2.77	0.41
1:C:276:LEU:CD2	1:C:278:LYS:HE2	2.50	0.40
1:C:464:GLN:NE2	1:C:468:ARG:HH12	2.13	0.40
1:A:162:VAL:HG13	1:A:176:ILE:HG12	2.03	0.40
1:A:275:SER:HA	1:A:285:LEU:HD23	2.03	0.40
1:A:294:THR:O	1:A:295:ARG:HD2	2.20	0.40
1:A:464:GLN:H	1:A:466:GLY:H	1.69	0.40
1:B:420:GLN:HG3	1:B:423:ALA:C	2.46	0.40
1:C:145:LEU:HB3	1:C:146:SER:H	1.53	0.40
1:C:165:VAL:HA	1:C:168:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:HZ3	1:C:316:LEU:HB3	1.87	0.40
1:A:211:ARG:HA	1:A:211:ARG:HD2	1.81	0.40
1:A:323:GLU:O	1:A:328:ARG:NH1	2.54	0.40
1:A:458:LYS:O	1:A:460:VAL:HG22	2.22	0.40
1:B:137:PHE:O	1:B:141:VAL:HG13	2.21	0.40
1:C:134:PHE:O	1:C:135:LEU:HD13	2.20	0.40
1:C:261:GLU:OE1	1:C:469:LEU:HD11	2.22	0.40
1:C:313:SER:C	1:C:316:LEU:HD23	2.46	0.40
1:A:255:VAL:HG23	1:A:260:LEU:HD11	2.03	0.40
1:A:273:SER:HB3	2:A:601:BLR:O1A	2.21	0.40
1:C:190:GLU:HB2	1:C:192:ARG:HB2	2.02	0.40
1:C:297:VAL:HG23	1:C:301:VAL:CG1	2.50	0.40
1:C:322:ASN:O	1:C:492:TYR:OH	2.39	0.40
1:C:438:PHE:O	1:C:439:VAL:HB	2.21	0.40
1:C:450:VAL:HG21	1:C:452:TRP:CH2	2.57	0.40
1:A:175:ILE:HD12	1:A:175:ILE:O	2.20	0.40
1:C:100:ARG:HH22	1:C:104:VAL:C	2.28	0.40
1:C:164:GLU:O	1:C:165:VAL:C	2.64	0.40
1:C:187:VAL:HG21	1:C:202:LEU:C	2.46	0.40
1:C:339:LEU:CD2	1:C:343:ALA:HB3	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	503/515 (98%)	446 (89%)	44 (9%)	13 (3%)	4	6
1	B	503/515 (98%)	444 (88%)	39 (8%)	20 (4%)	2	3
1	C	498/515 (97%)	332 (67%)	122 (24%)	44 (9%)	0	0
All	All	1504/1545 (97%)	1222 (81%)	205 (14%)	77 (5%)	1	2

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	44	VAL
1	A	389	THR
1	A	458	LYS
1	B	14	ASP
1	B	328	ARG
1	B	375	ARG
1	B	385	ASP
1	B	448	GLN
1	B	484	GLY
1	C	90	LYS
1	C	93	ASN
1	C	145	LEU
1	C	313	SER
1	C	392	ILE
1	C	414	PRO
1	C	421	GLU
1	C	439	VAL
1	C	447	VAL
1	C	470	HIS
1	A	395	LEU
1	A	448	GLN
1	A	510	GLN
1	B	128	HIS
1	B	383	PRO
1	B	463	ASP
1	C	20	ARG
1	C	94	PRO
1	C	102	ASP
1	C	282	LEU
1	C	358	GLY
1	C	429	PHE
1	C	431	MET
1	C	456	PRO
1	C	462	PHE
1	C	468	ARG
1	C	471	PRO
1	A	128	HIS
1	A	386	GLU
1	A	394	TRP
1	A	400	GLY
1	A	463	ASP

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Mol	Chain	Res	Type
1	B	195	ARG
1	B	316	LEU
1	B	384	SER
1	B	398	ARG
1	C	152	ARG
1	C	174	ALA
1	C	307	PHE
1	C	417	GLN
1	B	323	GLU
1	B	324	ASP
1	B	464	GLN
1	C	103	GLY
1	C	200	LEU
1	C	364	HIS
1	C	464	GLN
1	A	12	GLU
1	C	169	THR
1	C	226	PRO
1	C	283	TRP
1	C	340	GLU
1	C	347	ASP
1	C	444	PRO
1	C	461	GLU
1	C	467	PRO
1	B	399	THR
1	C	312	MET
1	C	460	VAL
1	C	465	GLY
1	B	22	PRO
1	B	378	VAL
1	C	26	PRO
1	C	73	GLU
1	C	79	PRO
1	C	144	GLY
1	B	434	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/427 (98%)	415 (99%)	4 (1%)	68	81
1	B	419/427 (98%)	412 (98%)	7 (2%)	53	73
1	C	414/427 (97%)	410 (99%)	4 (1%)	68	81
All	All	1252/1281 (98%)	1237 (99%)	15 (1%)	63	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	127	SER
1	A	211	ARG
1	A	322	ASN
1	B	73	GLU
1	B	141	VAL
1	B	207	SER
1	B	350	SER
1	B	377	THR
1	B	384	SER
1	B	495	GLU
1	C	83	ASP
1	C	136	SER
1	C	384	SER
1	C	453	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	30	GLN
1	A	113	HIS
1	B	91	GLN
1	B	269	GLN
1	B	335	HIS
1	B	355	GLN
1	C	17	ASN
1	C	58	ASN
1	C	364	HIS
1	C	417	GLN
1	C	510	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	BLR	B	601	1	46,46,46	3.54	22 (47%)	66,67,67	1.72	18 (27%)
2	BLR	C	601	1	46,46,46	3.56	21 (45%)	66,67,67	1.63	14 (21%)
2	BLR	A	601	1	46,46,46	3.55	22 (47%)	66,67,67	1.73	13 (19%)

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	BLR	B	601	1	-	10/26/58/58	0/4/4/4
2	BLR	C	601	1	-	11/26/58/58	0/4/4/4
2	BLR	A	601	1	-	7/26/58/58	0/4/4/4

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	BLR	C1B-NB	9.56	1.54	1.37
2	C	601	BLR	C4C-NC	9.53	1.54	1.37
2	A	601	BLR	C4C-NC	9.19	1.53	1.37
2	B	601	BLR	C1B-NB	8.86	1.52	1.37
2	B	601	BLR	C4C-NC	8.72	1.52	1.37
2	A	601	BLR	C1B-NB	8.65	1.52	1.37
2	A	601	BLR	C1D-ND	7.93	1.51	1.37
2	B	601	BLR	C4D-ND	7.74	1.53	1.37
2	A	601	BLR	C4D-ND	7.32	1.53	1.37
2	C	601	BLR	C1C-NC	6.95	1.54	1.38
2	B	601	BLR	C1D-ND	6.87	1.49	1.37
2	C	601	BLR	C4B-NB	6.80	1.53	1.38
2	C	601	BLR	C4D-ND	6.80	1.51	1.37
2	B	601	BLR	C1C-NC	6.79	1.53	1.38
2	A	601	BLR	C1C-NC	6.59	1.53	1.38
2	C	601	BLR	C1D-ND	6.52	1.48	1.37
2	A	601	BLR	C4B-NB	6.33	1.52	1.38
2	C	601	BLR	C4D-C3D	6.27	1.55	1.39
2	B	601	BLR	CHB-C4A	6.15	1.54	1.40
2	C	601	BLR	CHB-C4A	6.08	1.54	1.40
2	B	601	BLR	C4B-NB	5.86	1.51	1.38
2	A	601	BLR	C4D-C3D	5.65	1.53	1.39
2	A	601	BLR	CHD-C1D	5.49	1.52	1.40
2	B	601	BLR	CHD-C1D	5.41	1.52	1.40
2	B	601	BLR	C4D-C3D	5.29	1.52	1.39
2	A	601	BLR	CHB-C4A	5.14	1.52	1.40
2	C	601	BLR	CHD-C1D	4.83	1.51	1.40
2	B	601	BLR	CHA-C4D	-4.23	1.33	1.49
2	A	601	BLR	CHA-C4D	-4.20	1.33	1.49
2	C	601	BLR	CHA-C4D	-4.06	1.33	1.49
2	B	601	BLR	C3D-C2D	3.30	1.47	1.38
2	C	601	BLR	CHD-C4C	-3.19	1.30	1.37
2	A	601	BLR	OB-C4B	-3.14	1.17	1.23
2	B	601	BLR	C1D-C2D	3.14	1.49	1.41
2	B	601	BLR	OB-C4B	-3.07	1.17	1.23
2	A	601	BLR	C3C-C2C	3.02	1.43	1.37
2	A	601	BLR	OC-C1C	-3.01	1.17	1.23
2	A	601	BLR	CHB-C1B	-2.99	1.30	1.37
2	A	601	BLR	C3D-C2D	2.98	1.46	1.38
2	B	601	BLR	C1B-C2B	2.97	1.50	1.45
2	B	601	BLR	C3C-C2C	2.87	1.43	1.37
2	A	601	BLR	CHD-C4C	-2.85	1.31	1.37
2	B	601	BLR	CHD-C4C	-2.84	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	BLR	C3B-C2B	2.78	1.42	1.37
2	B	601	BLR	OC-C1C	-2.77	1.18	1.23
2	C	601	BLR	C3C-C2C	2.69	1.42	1.37
2	C	601	BLR	C3D-C2D	2.67	1.45	1.38
2	B	601	BLR	C3C-C4C	2.61	1.50	1.45
2	A	601	BLR	C3B-C2B	2.55	1.42	1.37
2	B	601	BLR	CAC-C3C	2.53	1.54	1.47
2	C	601	BLR	OC-C1C	-2.51	1.18	1.23
2	B	601	BLR	C3B-C2B	2.50	1.42	1.37
2	A	601	BLR	CAC-C3C	2.50	1.54	1.47
2	B	601	BLR	CHB-C1B	-2.50	1.31	1.37
2	C	601	BLR	OB-C4B	-2.47	1.18	1.23
2	C	601	BLR	C1B-C2B	2.46	1.49	1.45
2	C	601	BLR	CHB-C1B	-2.38	1.32	1.37
2	A	601	BLR	C1D-C2D	2.36	1.47	1.41
2	C	601	BLR	C1D-C2D	2.33	1.47	1.41
2	C	601	BLR	CAC-C3C	2.30	1.53	1.47
2	A	601	BLR	C2A-C3A	-2.21	1.33	1.38
2	C	601	BLR	CAB-C3B	2.20	1.53	1.47
2	B	601	BLR	CAB-C3B	2.18	1.53	1.47
2	A	601	BLR	C3C-C4C	2.13	1.49	1.45
2	A	601	BLR	CAB-C3B	2.13	1.53	1.47

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BLR	CHA-C4D-ND	5.55	133.32	122.04
2	A	601	BLR	CHA-C4D-ND	4.72	131.63	122.04
2	B	601	BLR	CHA-C4D-C3D	-4.41	121.64	130.07
2	C	601	BLR	C4C-NC-C1C	-4.22	105.48	110.66
2	A	601	BLR	CHD-C1D-C2D	-3.95	117.86	127.53
2	A	601	BLR	CMA-C3A-C4A	3.72	131.02	125.62
2	A	601	BLR	CHA-C4D-C3D	-3.64	123.12	130.07
2	C	601	BLR	CHD-C1D-C2D	-3.37	119.27	127.53
2	A	601	BLR	C4C-NC-C1C	-3.37	106.53	110.66
2	B	601	BLR	C4D-CHA-C1A	3.18	128.01	115.77
2	C	601	BLR	CAD-C3D-C2D	-3.09	120.14	127.07
2	A	601	BLR	CHD-C1D-ND	3.05	132.17	125.29
2	C	601	BLR	C1B-NB-C4B	-2.98	107.01	110.66
2	B	601	BLR	CAD-CBD-CGD	-2.94	105.88	113.67
2	C	601	BLR	C3B-C2B-C1B	2.89	111.14	107.92
2	A	601	BLR	C3B-C2B-C1B	2.88	111.13	107.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BLR	CHA-C1A-C2A	-2.88	124.56	130.07
2	B	601	BLR	CHD-C1D-C2D	-2.76	120.77	127.53
2	B	601	BLR	C4C-NC-C1C	-2.75	107.29	110.66
2	A	601	BLR	C4D-CHA-C1A	2.74	126.34	115.77
2	B	601	BLR	CMA-C3A-C4A	2.72	129.58	125.62
2	C	601	BLR	CHA-C4D-ND	2.72	127.57	122.04
2	A	601	BLR	CAA-C2A-C3A	-2.72	120.97	127.07
2	B	601	BLR	C1B-NB-C4B	-2.53	107.55	110.66
2	C	601	BLR	C4D-CHA-C1A	2.52	125.48	115.77
2	C	601	BLR	O1D-CGD-CBD	2.51	121.93	114.00
2	A	601	BLR	C1B-NB-C4B	-2.43	107.67	110.66
2	B	601	BLR	CHB-C4A-NA	-2.43	119.80	125.29
2	C	601	BLR	CHB-C1B-NB	2.36	131.10	126.06
2	B	601	BLR	O1A-CGA-O2A	-2.31	117.39	123.33
2	C	601	BLR	CHD-C1D-ND	2.30	130.48	125.29
2	C	601	BLR	CHA-C1A-NA	2.29	126.69	122.04
2	B	601	BLR	CHB-C4A-C3A	2.28	133.12	127.53
2	A	601	BLR	C4D-C3D-C2D	2.28	110.05	107.33
2	A	601	BLR	O1A-CGA-CBA	2.25	121.12	114.00
2	B	601	BLR	CHA-C1A-NA	2.24	126.60	122.04
2	B	601	BLR	CMB-C2B-C1B	2.23	126.87	124.16
2	B	601	BLR	CHD-C1D-ND	2.21	130.29	125.29
2	C	601	BLR	C3D-C4D-ND	-2.20	104.61	107.77
2	B	601	BLR	CMB-C2B-C3B	-2.15	123.22	128.43
2	A	601	BLR	O1D-CGD-CBD	2.09	120.61	114.00
2	B	601	BLR	C4D-C3D-C2D	2.08	109.81	107.33
2	B	601	BLR	C4B-C3B-C2B	2.06	110.57	107.92
2	C	601	BLR	C2D-C1D-ND	2.05	110.23	107.43
2	C	601	BLR	CMA-C3A-C4A	2.02	128.55	125.62

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	BLR	C2C-C3C-CAC-CBC
2	B	601	BLR	C4C-C3C-CAC-CBC
2	C	601	BLR	NA-C4A-CHB-C1B
2	C	601	BLR	C3A-C4A-CHB-C1B
2	C	601	BLR	C2A-CAA-CBA-CGA
2	C	601	BLR	C3D-CAD-CBD-CGD
2	A	601	BLR	NA-C4A-CHB-C1B
2	B	601	BLR	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
2	A	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C3A-C4A-CHB-C1B
2	C	601	BLR	NC-C4C-CHD-C1D
2	C	601	BLR	NB-C1B-CHB-C4A
2	C	601	BLR	C3C-C4C-CHD-C1D
2	C	601	BLR	C2B-C1B-CHB-C4A
2	B	601	BLR	NB-C1B-CHB-C4A
2	B	601	BLR	CAA-CBA-CGA-O2A
2	B	601	BLR	CAD-CBD-CGD-O1D
2	B	601	BLR	CAD-CBD-CGD-O2D
2	C	601	BLR	CAD-CBD-CGD-O2D
2	A	601	BLR	CAD-CBD-CGD-O2D
2	A	601	BLR	CAA-CBA-CGA-O2A
2	A	601	BLR	NB-C1B-CHB-C4A
2	C	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAA-CBA-CGA-O1A
2	B	601	BLR	CAA-CBA-CGA-O1A
2	A	601	BLR	CAD-CBD-CGD-O1D
2	B	601	BLR	C2B-C1B-CHB-C4A
2	C	601	BLR	CAA-CBA-CGA-O2A

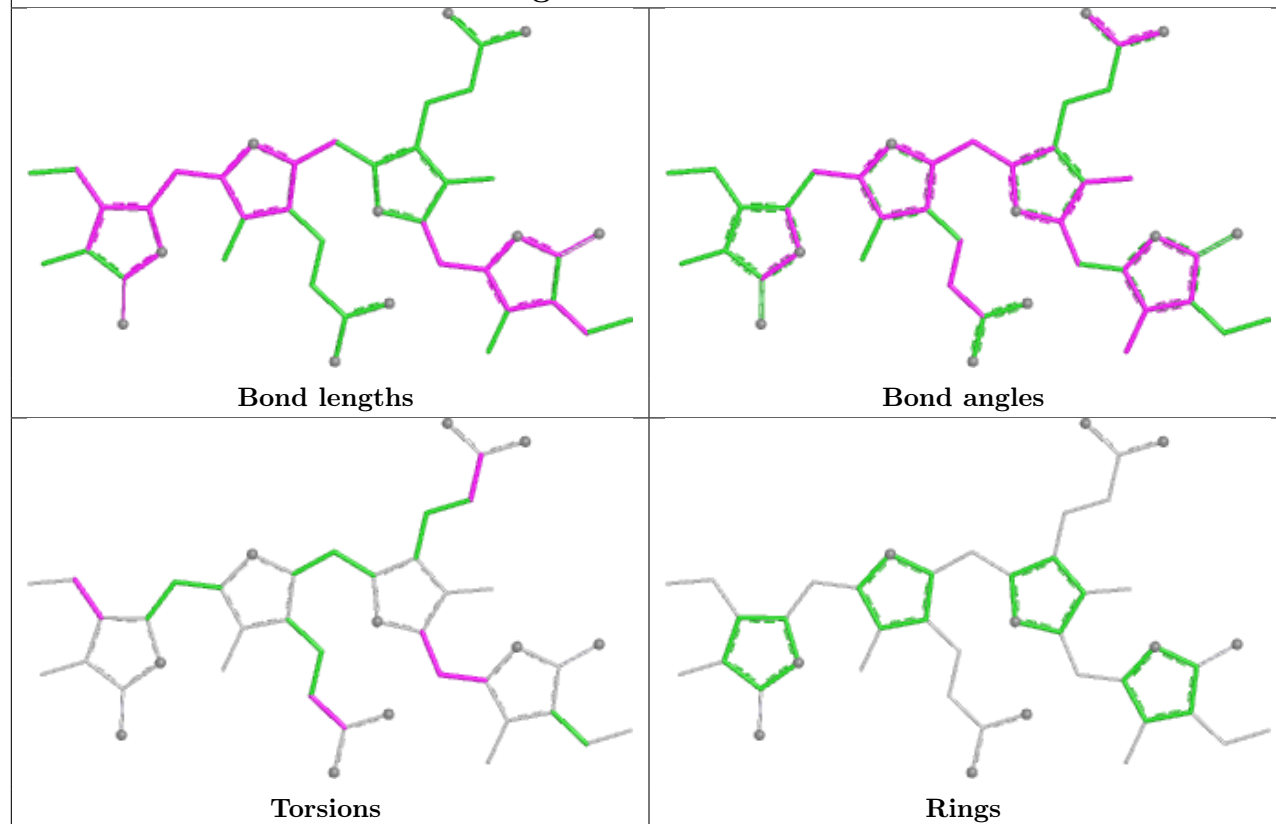
There are no ring outliers.

3 monomers are involved in 21 short contacts:

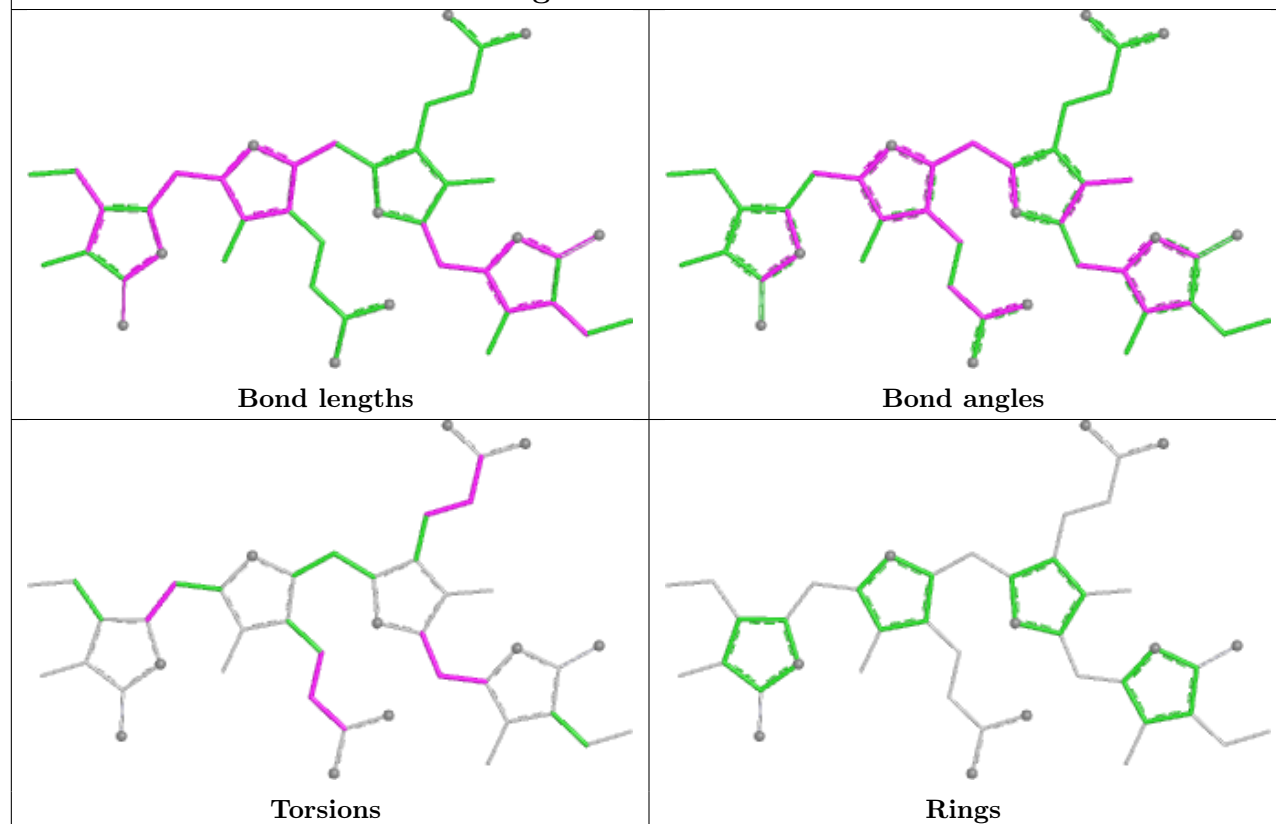
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BLR	3	0
2	C	601	BLR	14	0
2	A	601	BLR	4	0

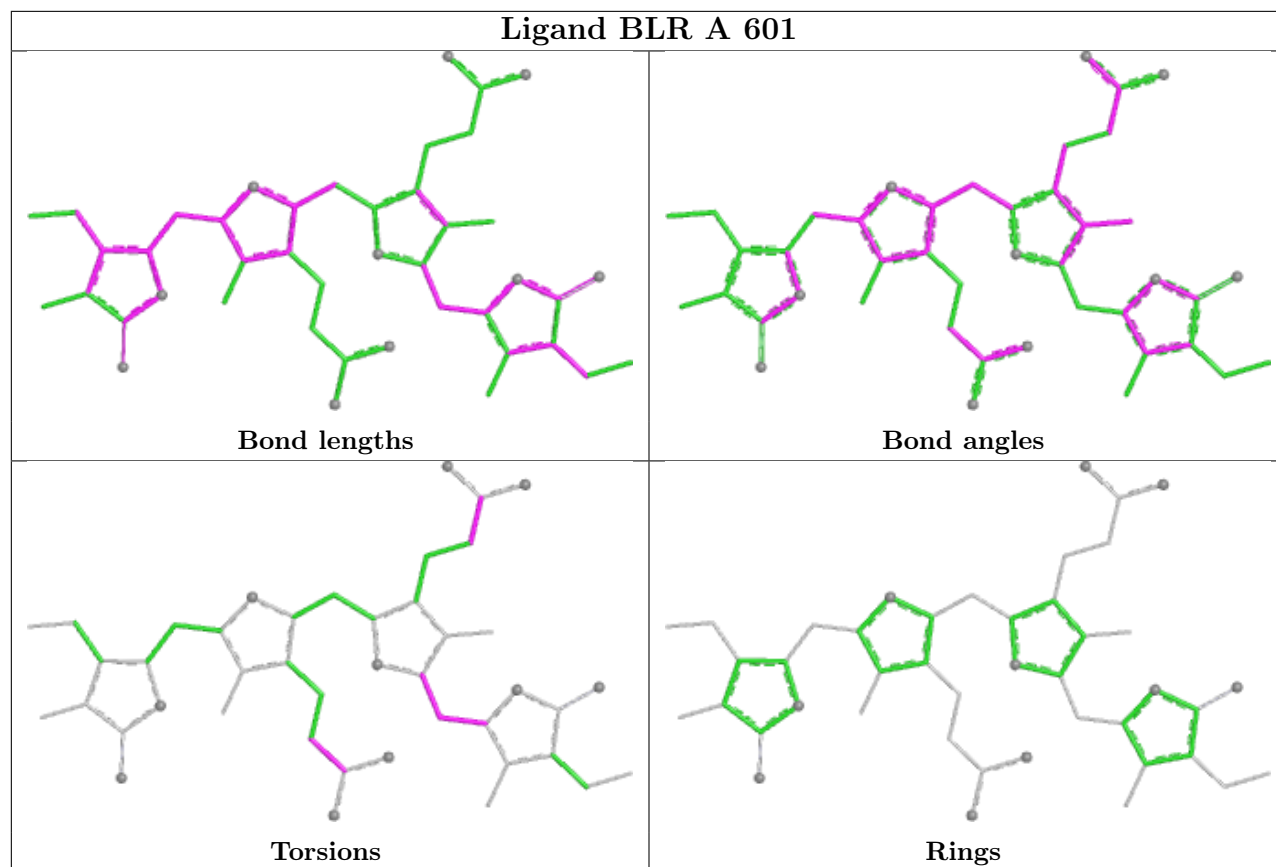
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand BLR B 601



Ligand BLR C 601





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	505/515 (98%)	-0.02	8 (1%) 70 66	35, 64, 99, 162	0
1	B	505/515 (98%)	0.03	8 (1%) 70 66	35, 69, 109, 135	1 (0%)
1	C	500/515 (97%)	1.19	105 (21%) 2 1	54, 106, 209, 230	3 (0%)
All	All	1510/1545 (97%)	0.40	121 (8%) 18 14	35, 74, 189, 230	4 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	ALA	6.0
1	C	439	VAL	5.4
1	C	338	LEU	5.4
1	B	424	ALA	5.2
1	C	307	PHE	5.1
1	C	441	TRP	4.4
1	C	440	LEU	4.4
1	B	425	GLY	4.4
1	C	409	LEU	4.2
1	C	334	ILE	4.1
1	C	424	ALA	4.0
1	C	316	LEU	4.0
1	C	456	PRO	4.0
1	C	315	LEU	3.9
1	C	186	SER	3.9
1	C	311	VAL	3.9
1	C	515	LEU	3.8
1	C	283	TRP	3.8
1	C	306	GLU	3.8
1	C	339	LEU	3.8
1	C	329	ILE	3.7
1	C	352	LEU	3.6
1	C	428	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	482	VAL	3.6
1	C	500	LEU	3.6
1	C	363	VAL	3.6
1	C	457	THR	3.5
1	C	187	VAL	3.4
1	C	388	LEU	3.4
1	C	391	LEU	3.3
1	C	132	VAL	3.3
1	C	404	PHE	3.2
1	C	89	LEU	3.2
1	C	504	ILE	3.2
1	C	188	ILE	3.1
1	C	204	PHE	3.1
1	A	459	ALA	3.1
1	C	359	LEU	3.1
1	C	318	ALA	3.1
1	C	154	LEU	3.1
1	C	191	ALA	3.0
1	C	426	LEU	3.0
1	C	406	THR	3.0
1	C	157	LEU	3.0
1	C	297	VAL	2.9
1	A	13	VAL	2.9
1	C	203	HIS	2.9
1	C	326	ASP	2.8
1	C	274	ILE	2.8
1	C	205	PRO	2.8
1	C	358	GLY	2.8
1	C	403	VAL	2.8
1	C	422	VAL	2.8
1	C	494	VAL	2.8
1	C	402	GLY	2.8
1	C	418	ALA	2.8
1	C	282	LEU	2.7
1	C	165	VAL	2.7
1	C	405	CYS	2.7
1	C	427	MET	2.7
1	C	373	HIS	2.7
1	C	286	ILE	2.7
1	C	429	PHE	2.7
1	B	515	LEU	2.7
1	C	275	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	277	MET	2.6
1	C	309	GLY	2.6
1	C	371	HIS	2.6
1	C	313	SER	2.6
1	C	143	ASP	2.6
1	A	16	THR	2.5
1	C	453	SER	2.5
1	C	383	PRO	2.5
1	C	337	ALA	2.5
1	C	489	TRP	2.5
1	C	285	LEU	2.4
1	C	492	TYR	2.4
1	C	498	SER	2.4
1	C	479	LYS	2.4
1	C	481	THR	2.4
1	C	353	ALA	2.4
1	C	462	PHE	2.4
1	C	179	PHE	2.4
1	C	222	LEU	2.3
1	C	413	TYR	2.3
1	C	380	GLY	2.3
1	C	442	PHE	2.3
1	C	452	TRP	2.3
1	A	462	PHE	2.3
1	C	438	PHE	2.3
1	C	336	ALA	2.3
1	A	399	THR	2.3
1	A	103	GLY	2.3
1	A	460	VAL	2.3
1	C	496	ALA	2.3
1	C	420	GLN	2.3
1	C	291	VAL	2.3
1	C	176	ILE	2.2
1	C	491	ALA	2.2
1	A	50	GLU	2.2
1	B	400	GLY	2.2
1	C	387	ALA	2.2
1	C	430	SER	2.2
1	B	383	PRO	2.2
1	B	379	LEU	2.2
1	C	314	SER	2.2
1	C	153	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	301	VAL	2.2
1	C	171	PHE	2.2
1	B	61	GLU	2.1
1	C	317	ALA	2.1
1	C	280	GLY	2.1
1	B	392	ILE	2.1
1	C	162	VAL	2.1
1	C	170	GLY	2.1
1	C	101	VAL	2.1
1	C	407	ASP	2.0
1	C	512	SER	2.0
1	C	183	TRP	2.0
1	C	360	LEU	2.0
1	C	142	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

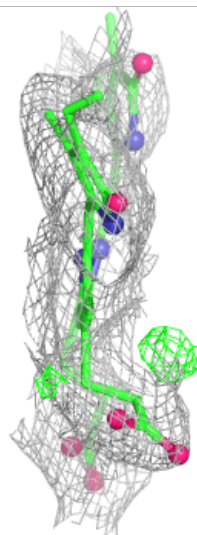
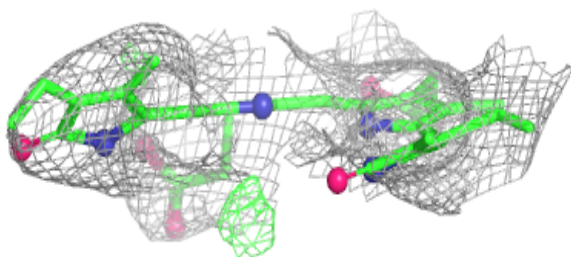
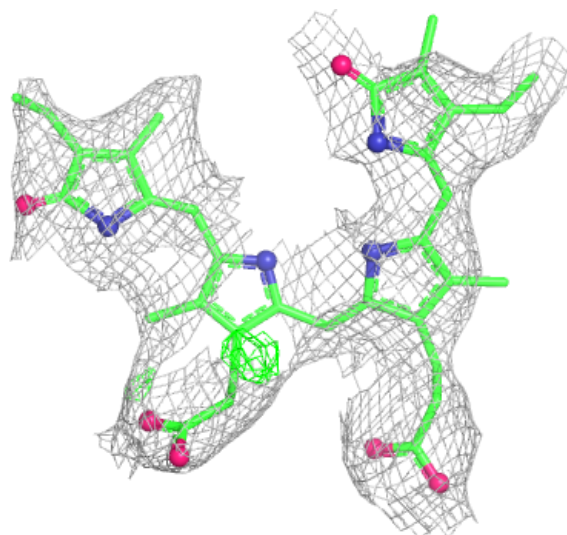
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BLR	C	601	43/43	0.89	0.13	86,97,113,118	0
2	BLR	A	601	43/43	0.95	0.09	47,60,78,94	1
2	BLR	B	601	43/43	0.96	0.08	43,51,63,67	1

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.

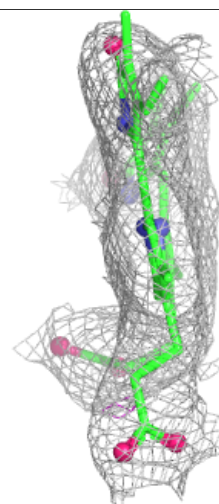
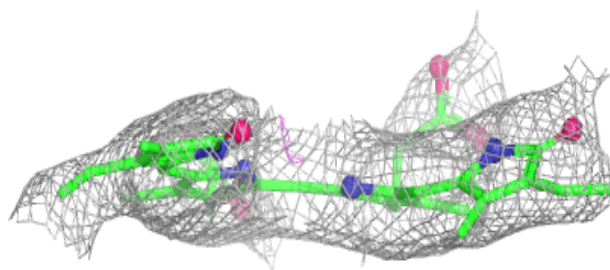
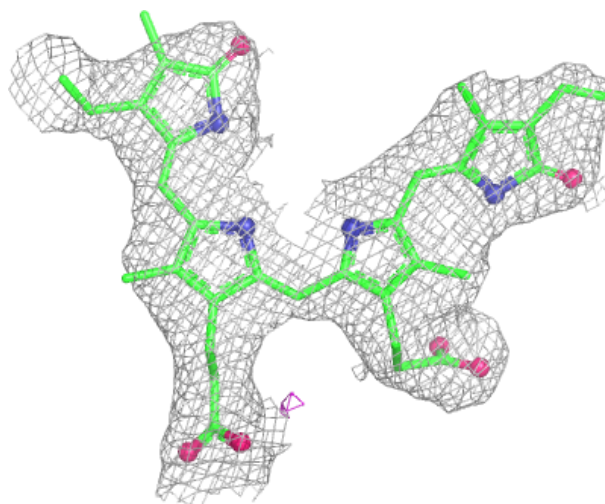
Electron density around BLR C 601:

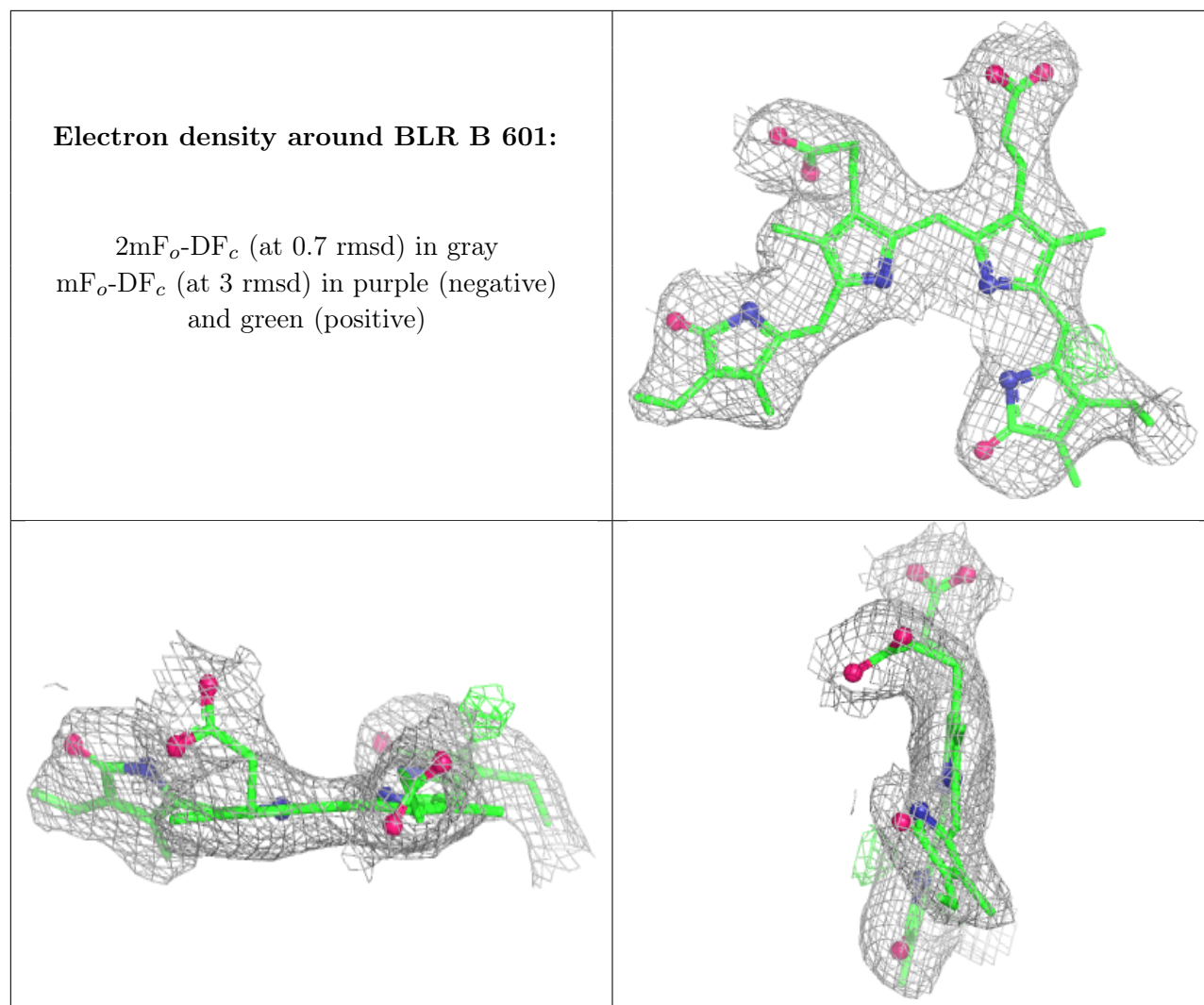
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLR A 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 ⓘ

There are no such residues in this entry.