Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 07:41 PM EDT

PDB ID	:	6BAY
Title	:	Stigmatella aurantiaca bacterial phytochrome P1, PAS-GAF-PHY T289H mutant, room temperature structure
Authors	:	Schmidt, M.; Stojkovic, E.
Deposited on	:	2017-10-16
Resolution	:	3.15 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:

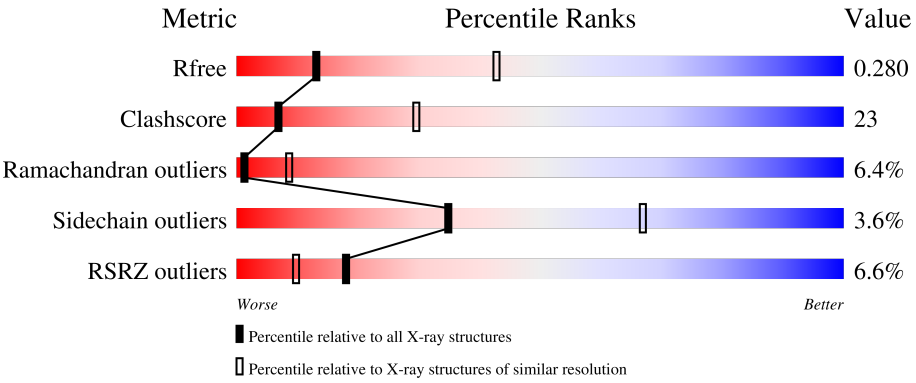
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	515	2% 63% 31%
1	B	515	6% 62% 32%
1	C	515	16% 41% 45% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12034 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.

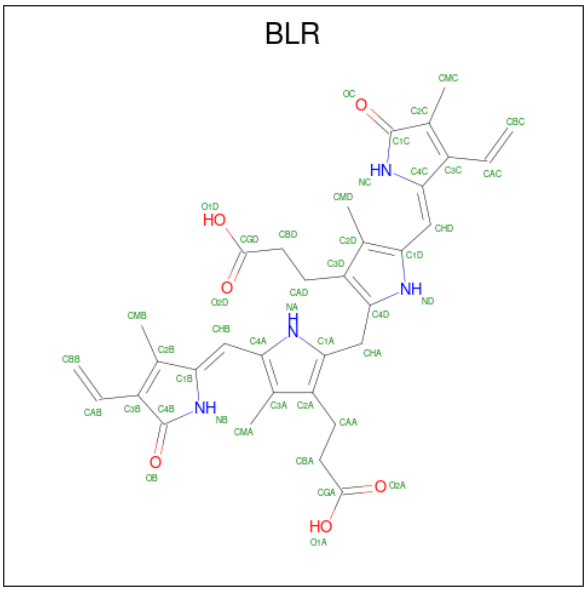
- Molecule 1 is a protein called Photoreceptor-histidine kinase BphP.

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 (three-letter code: BLR) (formula: $C_{33}H_{36}N_4O_6$).



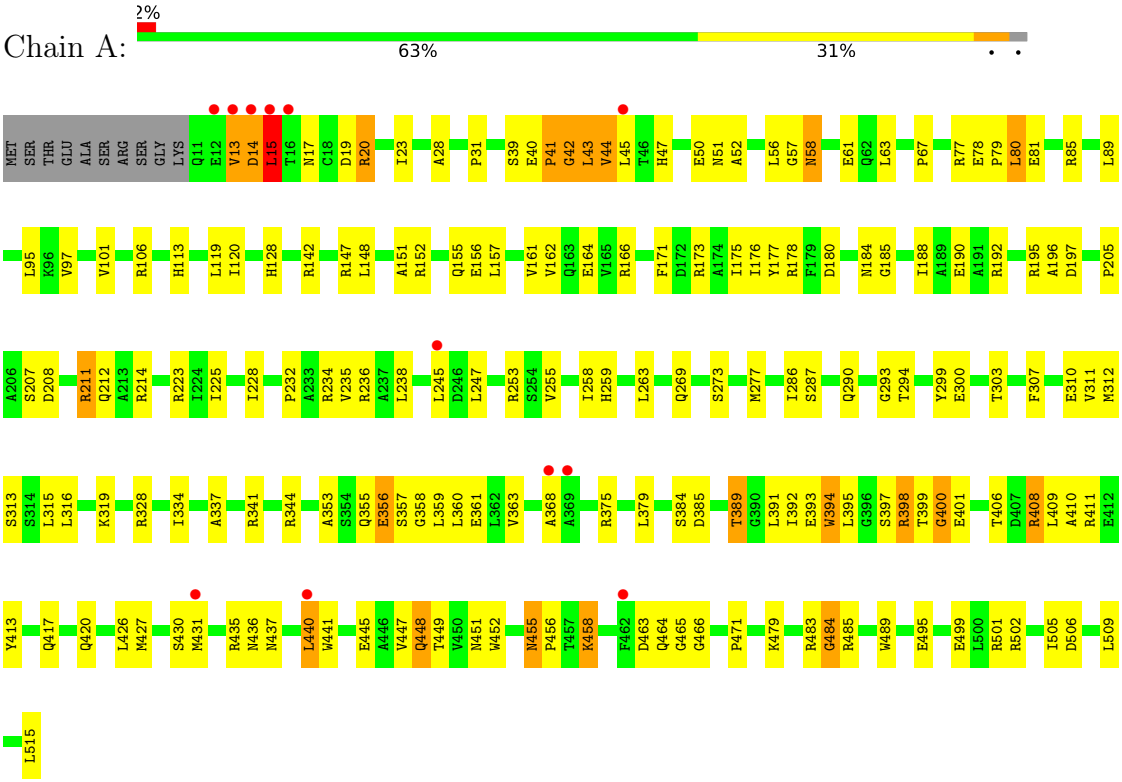
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 43 33 4 6	0	0
2	B	1	Total C N O 43 33 4 6	0	0
2	C	1	Total C N O 43 33 4 6	0	0

3 Residue-property plots (i)

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

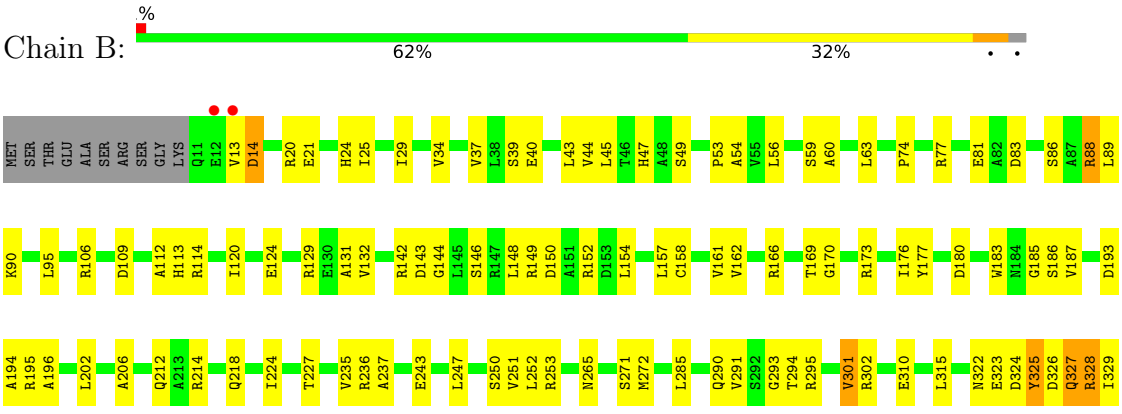
• Molecule 1: Photoreceptor-histidine kinase BphP

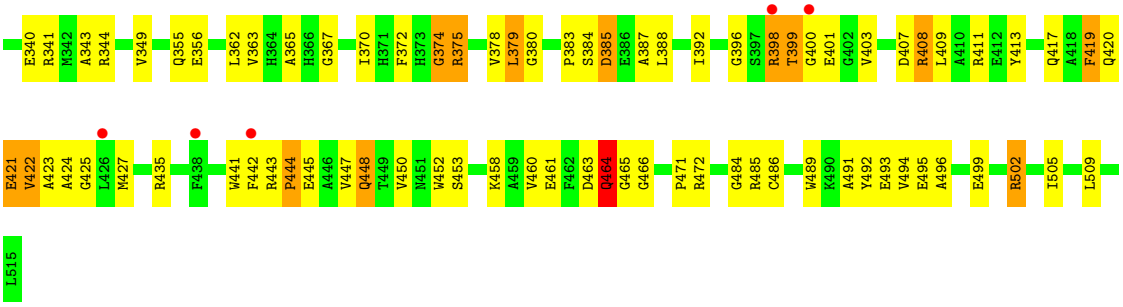
Chain A:



• Molecule 1: Photoreceptor-histidine kinase BphP

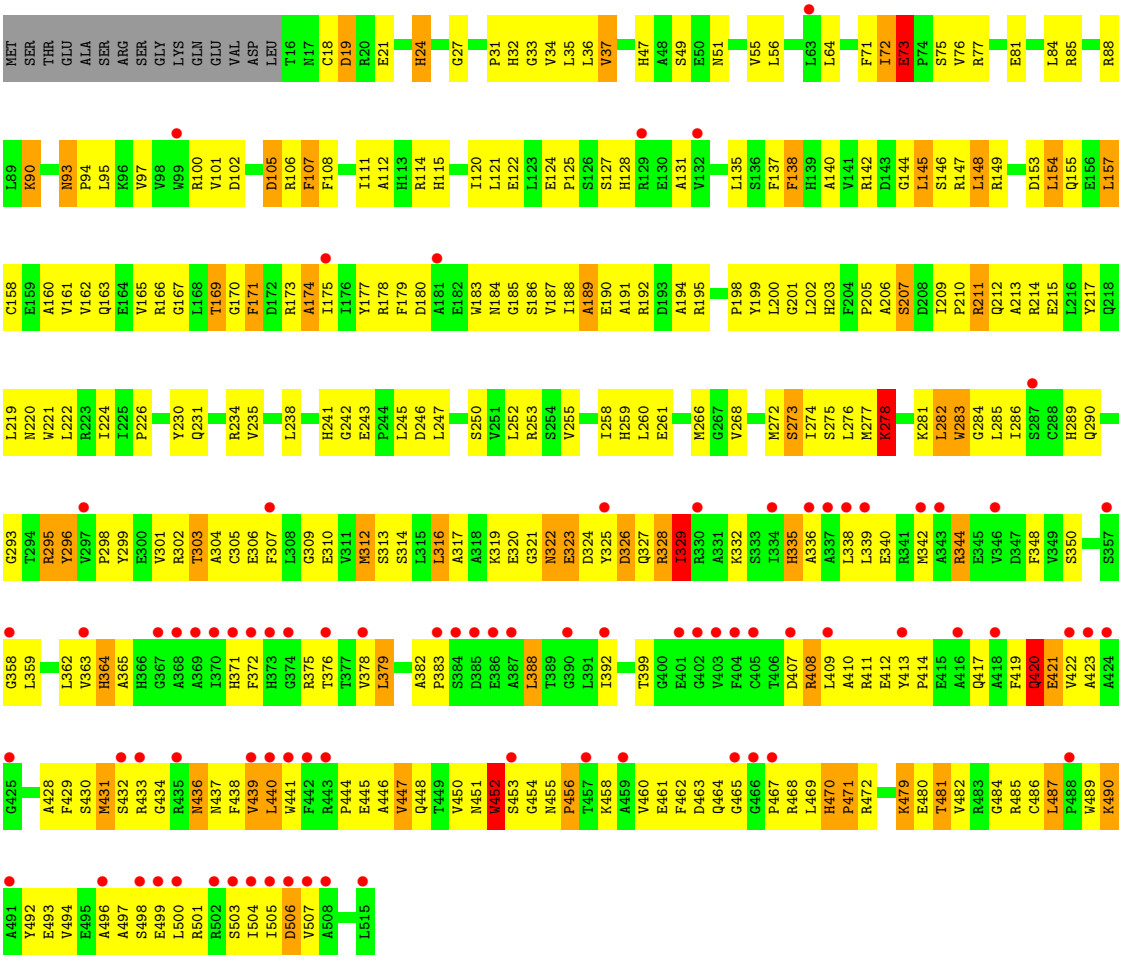
Chain B:





• Molecule 1: Photoreceptor-histidine kinase BphP

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.23Å 84.23Å 477.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.80 – 3.15 57.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (53.80-3.15) 89.0 (57.99-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.222 , 0.282 0.220 , 0.280	Depositor DCC
R_{free} test set	2047 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	104.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 85.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.128 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12034	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.65	4/4075 (0.1%)	0.84	11/5529 (0.2%)
1	B	0.61	2/4075 (0.0%)	0.81	5/5529 (0.1%)
1	C	0.53	2/4034 (0.0%)	0.80	9/5473 (0.2%)
All	All	0.60	8/12184 (0.1%)	0.82	25/16531 (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	2
1	C	0	3
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	487	LEU	C-N	6.71	1.47	1.34
1	A	408	ARG	NE-CZ	-5.91	1.25	1.33
1	A	408	ARG	CD-NE	-5.82	1.36	1.46
1	A	408	ARG	CZ-NH2	-5.76	1.25	1.33
1	A	408	ARG	CZ-NH1	-5.52	1.25	1.33
1	C	37	VAL	CB-CG2	-5.51	1.41	1.52
1	B	20	ARG	C-N	5.49	1.46	1.34
1	B	158	CYS	CB-SG	-5.11	1.73	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	413	TYR	C-N-CD	-8.82	101.20	120.60
1	A	43	LEU	CA-CB-CG	7.61	132.80	115.30
1	A	43	LEU	CB-CG-CD2	7.06	123.00	111.00
1	B	315	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	C	157	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	15	LEU	CA-CB-CG	6.20	129.57	115.30
1	C	148	LEU	CA-CB-CG	-6.09	101.29	115.30
1	A	238	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	219	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	56	LEU	CA-CB-CG	5.93	128.94	115.30
1	B	180	ASP	CB-CG-OD1	5.88	123.60	118.30
1	C	329	ILE	C-N-CA	-5.71	107.43	121.70
1	A	95	LEU	CA-CB-CG	5.60	128.17	115.30
1	A	440	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	154	LEU	CA-CB-CG	5.40	127.73	115.30
1	C	316	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	56	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	C	413	TYR	C-N-CA	5.26	144.11	122.00
1	C	388	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	45	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	315	LEU	CB-CG-CD2	-5.23	102.12	111.00
1	B	106	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	301	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	A	13	VAL	C-N-CA	5.14	134.55	121.70
1	B	374	GLY	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	GLY	Peptide
1	B	322	ASN	Peptide
1	B	422	VAL	Peptide
1	C	273	SER	Peptide
1	C	420	GLN	Peptide
1	C	490	LYS	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	3925	145	0
1	B	3982	0	3925	144	0
1	C	3941	0	3887	267	0
2	A	43	0	32	5	0
2	B	43	0	33	5	0
2	C	43	0	32	10	0
All	All	12034	0	11834	551	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 23.

All (551) 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:B:492:TYR:HA	1:B:495:GLU:OE2	1.47	1.14
1:A:173:ARG:NH2	1:A:197:ASP:O	1.90	1.04
1:C:122:GLU:OE1	1:C:250:SER:OG	1.77	1.03
1:C:430:SER:HB2	1:C:439:VAL:HG12	1.45	0.98
1:B:492:TYR:CA	1:B:495:GLU:OE2	2.14	0.94
1:B:492:TYR:HA	1:B:495:GLU:CD	1.86	0.94
1:C:339:LEU:HD22	1:C:507:VAL:HG21	1.52	0.91
1:A:13:VAL:HA	1:A:14:ASP:HB2	1.51	0.91
1:B:422:VAL:HG22	1:B:425:GLY:HA2	1.51	0.91
1:C:222:LEU:HD21	1:C:302:ARG:HD2	1.54	0.90
1:A:394:TRP:HB2	1:A:398:ARG:HB2	1.56	0.87
1:C:364:HIS:ND1	1:C:493:GLU:OE2	2.08	0.87
1:C:224:ILE:HG22	1:C:272:MET:HG2	1.56	0.85
1:C:408:ARG:NH2	1:C:445:GLU:OE1	2.09	0.85
1:B:327:GLN:O	1:B:329:ILE:N	2.10	0.84
1:A:310:GLU:OE2	1:B:149:ARG:NH1	2.10	0.84
1:C:319:LYS:HA	1:C:322:ASN:HB2	1.58	0.83
1:A:277:MET:O	1:A:313:SER:HB3	1.81	0.80
1:C:408:ARG:O	1:C:417:GLN:NE2	2.14	0.80
1:B:177:TYR:CZ	1:B:185:GLY:HA3	2.17	0.79
1:C:408:ARG:NH2	1:C:421:GLU:OE2	2.16	0.78
1:A:394:TRP:HD1	1:A:398:ARG:CZ	1.97	0.77
1:C:211:ARG:O	1:C:212:GLN:NE2	2.18	0.76
1:B:458:LYS:HE3	1:B:461:GLU:HG2	1.68	0.76
1:A:44:VAL:H	1:A:67:PRO:HA	1.51	0.76
1:B:409:LEU:H	1:B:422:VAL:CG2	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ARG:HD3	1:C:90:LYS:HD3	1.67	0.75
1:A:394:TRP:O	1:A:398:ARG:NH1	2.20	0.75
1:C:100:ARG:NH2	1:C:105:ASP:OD1	2.20	0.75
1:C:447:VAL:HB	1:C:484:GLY:HA2	1.69	0.74
1:A:41:PRO:O	1:A:43:LEU:HD22	1.87	0.74
1:A:464:GLN:H	1:A:466:GLY:H	1.35	0.74
1:C:73:GLU:HB3	1:C:100:ARG:HE	1.53	0.74
1:C:303:THR:O	1:C:307:PHE:N	2.21	0.74
1:B:148:LEU:HD21	1:B:161:VAL:HG23	1.68	0.74
1:C:489:TRP:HB2	1:C:494:VAL:HG22	1.69	0.73
1:C:438:PHE:HB3	1:C:440:LEU:HD13	1.71	0.73
1:C:329:ILE:HG23	1:C:332:LYS:HE3	1.68	0.73
1:A:173:ARG:HG3	1:A:192:ARG:HB3	1.71	0.72
1:A:192:ARG:NH1	1:A:196:ALA:O	2.22	0.72
1:B:202:LEU:HD13	1:B:453:SER:HB2	1.71	0.72
1:A:151:ALA:O	1:A:319:LYS:NZ	2.18	0.72
1:A:307:PHE:HD1	1:B:149:ARG:HD3	1.52	0.72
1:C:73:GLU:OE2	1:C:75:SER:N	2.23	0.72
1:C:429:PHE:HB3	1:C:498:SER:HB3	1.70	0.72
1:C:73:GLU:OE1	1:C:76:VAL:HG22	1.90	0.71
1:C:166:ARG:NH1	1:C:191:ALA:O	2.24	0.71
1:B:491:ALA:O	1:B:495:GLU:OE2	2.08	0.71
1:C:339:LEU:HD13	1:C:507:VAL:HG11	1.73	0.71
1:A:175:ILE:HD11	1:A:287:SER:HB3	1.72	0.70
1:B:150:ASP:O	1:B:152:ARG:NH1	2.23	0.70
1:C:463:ASP:OD2	1:C:468:ARG:NH1	2.24	0.70
1:A:394:TRP:CD1	1:A:398:ARG:CZ	2.75	0.70
1:B:60:ALA:HB3	1:B:236:ARG:HD3	1.74	0.70
1:B:423:ALA:HA	1:B:444:PRO:C	2.11	0.70
1:B:374:GLY:HA3	1:B:375:ARG:HG2	1.74	0.69
1:B:453:SER:O	1:B:472:ARG:NH2	2.25	0.69
1:B:325:TYR:O	1:B:328:ARG:HB3	1.93	0.69
1:A:31:PRO:O	1:A:51:ASN:ND2	2.26	0.69
1:A:80:LEU:HD11	1:A:97:VAL:HG22	1.74	0.69
1:A:509:LEU:HD22	1:B:505:ILE:HG23	1.75	0.69
1:C:190:GLU:OE1	1:C:200:LEU:HG	1.93	0.69
1:C:124:GLU:OE2	1:C:302:ARG:NH2	2.26	0.69
1:C:73:GLU:HB3	1:C:100:ARG:NE	2.07	0.68
1:C:84:LEU:O	1:C:114:ARG:NH2	2.27	0.68
1:C:175:ILE:HD13	1:C:187:VAL:HG13	1.76	0.67
1:C:363:VAL:HA	1:C:493:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:VAL:HG23	1:C:482:VAL:HG22	1.75	0.67
1:B:420:GLN:O	1:B:423:ALA:HB3	1.95	0.67
1:C:21:GLU:N	1:C:212:GLN:OE1	2.25	0.67
1:C:278:LYS:HE3	1:C:317:ALA:HB2	1.76	0.67
1:C:258:ILE:HG22	1:C:469:LEU:HD12	1.76	0.67
1:C:471:PRO:HB3	2:C:601:BLR:H22	1.77	0.66
1:C:32:HIS:CE1	1:C:226:PRO:HG3	2.31	0.66
1:C:224:ILE:HG21	1:C:302:ARG:HD3	1.76	0.66
1:B:193:ASP:O	1:B:195:ARG:N	2.30	0.65
1:C:179:PHE:HD2	1:C:284:GLY:HA2	1.61	0.65
1:C:19:ASP:HA	1:C:212:GLN:HG2	1.78	0.65
1:B:166:ARG:O	1:B:170:GLY:N	2.30	0.65
1:B:177:TYR:CE1	1:B:185:GLY:HA3	2.31	0.65
1:B:409:LEU:H	1:B:422:VAL:HG21	1.59	0.65
1:C:107:PHE:HB3	1:C:127:SER:HB3	1.78	0.65
1:A:178:ARG:HB2	1:A:188:ILE:HD13	1.79	0.65
1:C:190:GLU:OE2	1:C:199:TYR:N	2.29	0.65
1:C:450:VAL:O	1:C:480:GLU:HB3	1.96	0.65
1:C:255:VAL:HG23	2:C:601:BLR:CGD	2.26	0.64
1:C:276:LEU:HD13	1:C:277:MET:N	2.12	0.64
1:C:49:SER:HA	1:C:235:VAL:HA	1.78	0.64
1:A:394:TRP:HB2	1:A:398:ARG:CB	2.26	0.64
1:A:61:GLU:N	1:A:61:GLU:OE1	2.31	0.63
1:A:307:PHE:CD1	1:B:149:ARG:HD3	2.33	0.63
1:C:175:ILE:CD1	1:C:187:VAL:HG13	2.29	0.63
1:B:43:LEU:HD12	1:B:81:GLU:HG2	1.81	0.63
1:C:327:GLN:NE2	1:C:493:GLU:HB2	2.13	0.63
1:A:177:TYR:CZ	1:A:185:GLY:HA3	2.34	0.63
1:B:109:ASP:OD2	1:B:129:ARG:NH1	2.32	0.63
1:C:147:ARG:HE	1:C:160:ALA:HB1	1.64	0.63
1:A:247:LEU:O	1:A:253:ARG:HD3	1.98	0.62
1:C:277:MET:HA	1:C:283:TRP:H	1.63	0.62
1:A:42:GLY:O	1:A:43:LEU:HD23	2.00	0.62
1:C:501:ARG:HH22	1:C:505:ILE:HD13	1.64	0.62
1:A:15:LEU:HD12	1:A:20:ARG:HH11	1.64	0.62
1:B:45:LEU:HD22	1:B:63:LEU:HB3	1.79	0.62
1:B:423:ALA:HB2	1:B:445:GLU:HB2	1.81	0.62
1:B:13:VAL:HA	1:B:14:ASP:CB	2.30	0.62
1:A:253:ARG:HH22	2:A:601:BLR:CGD	2.13	0.62
1:B:464:GLN:HB2	1:B:465:GLY:HA3	1.80	0.62
1:B:195:ARG:HG2	1:B:291:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:TYR:OH	2:C:601:BLR:H33	1.99	0.61
1:B:86:SER:OG	1:B:88:ARG:HG3	1.99	0.61
1:C:201:GLY:O	1:C:451:ASN:ND2	2.27	0.61
1:B:169:THR:O	1:B:295:ARG:NH2	2.34	0.61
1:C:171:PHE:HB3	1:C:173:ARG:O	2.01	0.61
1:C:72:ILE:O	1:C:73:GLU:HG3	2.02	0.60
1:C:108:PHE:HA	1:C:125:PRO:HA	1.81	0.60
1:A:234:ARG:HH11	1:A:234:ARG:HB2	1.67	0.60
1:C:274:ILE:HD12	1:C:306:GLU:HA	1.83	0.60
1:C:439:VAL:HG13	1:C:497:ALA:HB1	1.84	0.60
1:B:143:ASP:O	1:B:146:SER:N	2.34	0.59
1:B:384:SER:HB2	1:B:388:LEU:HB2	1.84	0.59
1:B:407:ASP:O	1:B:485:ARG:HA	2.03	0.59
1:C:213:ALA:HB1	1:C:217:TYR:CZ	2.37	0.59
1:C:224:ILE:HD12	1:C:226:PRO:HD3	1.83	0.59
1:B:132:VAL:HG21	1:B:301:VAL:HG21	1.85	0.59
2:B:601:BLR:H4	2:B:601:BLR:NB	2.17	0.58
1:C:145:LEU:O	1:C:149:ARG:HG2	2.03	0.58
1:B:53:PRO:HG3	1:B:59:SER:HA	1.85	0.58
1:B:247:LEU:HD22	1:B:250:SER:OG	2.03	0.58
1:B:251:VAL:HG23	1:B:252:LEU:HG	1.85	0.58
1:B:409:LEU:H	1:B:422:VAL:HG23	1.69	0.58
1:A:299:TYR:CZ	1:A:303:THR:HG21	2.39	0.58
1:C:33:GLY:HA3	1:C:252:LEU:HD11	1.84	0.58
1:A:142:ARG:NH1	1:B:310:GLU:OE2	2.36	0.58
1:C:487:LEU:HB2	1:C:489:TRP:CD1	2.39	0.58
1:B:349:VAL:HG21	1:B:372:PHE:CG	2.38	0.58
1:C:342:MET:HG2	1:C:504:ILE:HG23	1.84	0.58
1:B:447:VAL:HG23	1:B:448:GLN:H	1.69	0.58
1:A:148:LEU:HD12	1:A:311:VAL:HG12	1.85	0.57
1:B:37:VAL:HG22	1:B:47:HIS:HB2	1.85	0.57
1:A:363:VAL:HG11	1:A:427:MET:CE	2.35	0.57
1:C:359:LEU:HD13	1:C:500:LEU:HD11	1.87	0.57
1:A:89:LEU:HD11	1:A:113:HIS:HA	1.86	0.57
1:B:60:ALA:CB	1:B:236:ARG:HD3	2.34	0.57
1:C:489:TRP:CE3	1:C:494:VAL:HG13	2.38	0.57
1:A:152:ARG:HG3	1:A:156:GLU:OE2	2.05	0.57
1:A:175:ILE:CD1	1:A:287:SER:HB3	2.35	0.57
1:C:302:ARG:O	1:C:306:GLU:N	2.20	0.57
1:B:443:ARG:HD2	1:B:489:TRP:CH2	2.39	0.57
1:C:184:ASN:OD1	1:C:206:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:NH1	2:C:601:BLR:O2D	2.37	0.57
1:B:356:GLU:HG3	1:B:379:LEU:HD21	1.87	0.57
1:B:214:ARG:O	1:B:218:GLN:HG3	2.04	0.57
1:A:44:VAL:N	1:A:67:PRO:HA	2.17	0.57
1:C:19:ASP:HB3	1:C:212:GLN:HE21	1.69	0.57
1:C:177:TYR:CZ	1:C:185:GLY:HA3	2.41	0.56
1:B:265:ASN:ND2	1:B:471:PRO:HG2	2.20	0.56
1:C:290:GLN:HG2	1:C:293:GLY:O	2.05	0.56
1:A:161:VAL:HG21	1:A:312:MET:HG3	1.88	0.56
1:C:371:HIS:CE1	1:C:388:LEU:HD23	2.40	0.56
1:B:422:VAL:HG13	1:B:425:GLY:HA3	1.88	0.56
1:C:295:ARG:HA	1:C:295:ARG:NE	2.20	0.56
1:C:470:HIS:ND1	1:C:471:PRO:HD2	2.21	0.56
1:C:174:ALA:HB3	1:C:191:ALA:HB3	1.88	0.56
1:C:73:GLU:OE1	1:C:76:VAL:N	2.25	0.55
1:C:73:GLU:CB	1:C:100:ARG:HE	2.18	0.55
1:A:234:ARG:HB2	1:A:234:ARG:NH1	2.22	0.55
1:A:401:GLU:OE1	1:A:501:ARG:NH2	2.39	0.55
1:C:335:HIS:HB2	1:C:362:LEU:HD22	1.86	0.55
1:B:132:VAL:HG21	1:B:301:VAL:CG2	2.36	0.55
1:B:21:GLU:HB3	1:B:212:GLN:HE21	1.71	0.55
1:C:137:PHE:CE2	1:C:301:VAL:HG22	2.42	0.55
1:C:275:SER:OG	1:C:282:LEU:HD21	2.07	0.55
1:B:89:LEU:HD21	1:B:112:ALA:HB3	1.88	0.55
1:C:148:LEU:HD21	1:C:161:VAL:HG11	1.87	0.55
1:C:179:PHE:CD2	1:C:284:GLY:HA2	2.41	0.55
1:A:445:GLU:OE2	1:A:484:GLY:N	2.38	0.55
1:C:137:PHE:HE2	1:C:301:VAL:HG22	1.72	0.55
1:C:332:LYS:HB2	1:C:335:HIS:HD2	1.72	0.55
1:A:408:ARG:NH1	1:A:485:ARG:HD3	2.22	0.55
1:C:362:LEU:HD21	1:C:500:LEU:HD13	1.89	0.55
1:A:455:ASN:ND2	1:A:458:LYS:HG3	2.22	0.55
1:B:464:GLN:CB	1:B:465:GLY:HA3	2.37	0.55
1:C:278:LYS:HG3	1:C:316:LEU:HG	1.88	0.55
1:C:432:SER:O	1:C:434:GLY:N	2.40	0.54
1:C:372:PHE:CE2	1:C:437:ASN:HB2	2.43	0.54
1:C:37:VAL:HG22	1:C:47:HIS:HB2	1.88	0.54
1:C:276:LEU:HD13	1:C:277:MET:H	1.70	0.54
1:C:338:LEU:HD23	1:C:504:ILE:HG12	1.90	0.54
1:C:101:VAL:HG11	1:C:106:ARG:NE	2.22	0.54
1:C:295:ARG:HA	1:C:295:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:HA	1:B:421:GLU:HG2	1.89	0.54
1:A:212:GLN:N	1:A:212:GLN:OE1	2.41	0.54
1:C:298:PRO:HD2	1:C:301:VAL:HB	1.90	0.54
1:A:410:ALA:HB1	1:A:417:GLN:OE1	2.08	0.54
1:C:177:TYR:CE2	1:C:185:GLY:HA3	2.43	0.54
1:A:358:GLY:O	1:A:361:GLU:N	2.41	0.54
1:B:24:HIS:CE1	1:B:25:ILE:HG13	2.43	0.54
1:B:365:ALA:HB1	1:B:442:PHE:O	2.08	0.54
1:C:276:LEU:HD21	1:C:312:MET:SD	2.47	0.53
1:B:24:HIS:ND1	1:B:25:ILE:HG23	2.23	0.53
1:C:124:GLU:CD	1:C:302:ARG:HH22	2.11	0.53
1:C:327:GLN:NE2	1:C:490:LYS:HB2	2.24	0.53
1:C:338:LEU:HD21	1:C:359:LEU:HD11	1.91	0.53
1:B:13:VAL:HA	1:B:14:ASP:HB3	1.90	0.53
1:C:221:TRP:NE1	1:C:277:MET:SD	2.81	0.53
1:A:259:HIS:NE2	1:A:263:LEU:HD11	2.23	0.53
1:A:505:ILE:HG23	1:B:509:LEU:HD22	1.90	0.53
1:C:320:GLU:N	1:C:321:GLY:HA3	2.24	0.53
1:C:332:LYS:HB2	1:C:335:HIS:CD2	2.44	0.53
1:C:448:GLN:O	1:C:482:VAL:HG11	2.08	0.53
1:C:259:HIS:NE2	2:C:601:BLR:H9	2.24	0.53
1:B:224:ILE:HG13	1:B:272:MET:HB2	1.91	0.52
1:B:187:VAL:CG2	2:B:601:BLR:H19	2.39	0.52
1:C:207:SER:O	1:C:207:SER:OG	2.26	0.52
1:A:23:ILE:HG21	2:A:601:BLR:H29	1.91	0.52
1:B:90:LYS:HE2	1:B:113:HIS:HA	1.92	0.52
1:C:147:ARG:HH21	1:C:160:ALA:HA	1.74	0.52
1:B:49:SER:HA	1:B:235:VAL:HA	1.91	0.52
1:B:83:ASP:O	1:B:86:SER:HB3	2.10	0.52
1:B:326:ASP:HA	1:B:327:GLN:O	2.10	0.52
1:A:393:GLU:HG3	1:A:413:TYR:CD1	2.45	0.52
1:A:447:VAL:HG13	1:A:448:GLN:H	1.74	0.52
1:B:464:GLN:HB2	1:B:465:GLY:CA	2.40	0.51
2:B:601:BLR:H21	2:B:601:BLR:H25	1.91	0.51
1:A:334:ILE:O	1:A:337:ALA:HB3	2.10	0.51
1:A:81:GLU:O	1:A:85:ARG:HD2	2.10	0.51
1:A:58:ASN:HB2	1:A:63:LEU:HD21	1.92	0.51
1:B:21:GLU:O	1:B:212:GLN:HG3	2.11	0.51
1:C:276:LEU:HB3	1:C:283:TRP:HE3	1.75	0.51
1:C:455:ASN:HB3	1:C:458:LYS:HB2	1.93	0.51
1:A:15:LEU:HB2	1:A:19:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:SER:OG	1:C:431:MET:N	2.44	0.51
1:A:483:ARG:O	1:A:485:ARG:N	2.43	0.51
1:B:290:GLN:HG2	1:B:293:GLY:O	2.10	0.51
1:C:448:GLN:C	1:C:482:VAL:HG11	2.31	0.51
1:A:42:GLY:HA3	1:A:85:ARG:HH21	1.76	0.51
1:B:349:VAL:HG13	1:B:370:ILE:HG21	1.92	0.51
1:B:422:VAL:HG12	1:B:486:CYS:HB3	1.93	0.51
1:B:495:GLU:O	1:B:499:GLU:HG2	2.11	0.51
1:C:111:ILE:HD12	1:C:299:TYR:CE1	2.47	0.51
1:C:328:ARG:O	1:C:332:LYS:HB3	2.11	0.51
1:C:365:ALA:CB	1:C:441:TRP:HB3	2.41	0.51
1:C:420:GLN:O	1:C:421:GLU:HB3	2.10	0.51
1:A:356:GLU:OE2	1:A:357:SER:N	2.44	0.50
1:B:326:ASP:HA	1:B:327:GLN:C	2.31	0.50
1:C:286:ILE:HD11	1:C:312:MET:HE1	1.91	0.50
1:A:228:ILE:HG12	1:A:269:GLN:O	2.11	0.50
1:A:451:ASN:OD1	1:A:479:LYS:HE2	2.10	0.50
1:C:210:PRO:HG2	1:C:212:GLN:HB2	1.93	0.50
1:C:327:GLN:OE1	1:C:490:LYS:HD3	2.11	0.50
1:A:15:LEU:HD12	1:A:20:ARG:NH1	2.26	0.50
1:A:223:ARG:NH2	1:A:273:SER:OG	2.39	0.50
1:C:135:LEU:HA	1:C:138:PHE:HB3	1.94	0.50
1:C:178:ARG:HD3	1:C:283:TRP:CE2	2.46	0.50
1:C:224:ILE:CG2	1:C:302:ARG:HD3	2.41	0.50
1:C:452:TRP:HZ2	1:C:456:PRO:N	2.08	0.50
1:A:78:GLU:N	1:A:78:GLU:CD	2.65	0.50
1:A:363:VAL:HG11	1:A:427:MET:HE3	1.92	0.50
1:C:276:LEU:O	1:C:283:TRP:N	2.44	0.50
1:C:335:HIS:O	1:C:503:SER:OG	2.22	0.50
1:C:446:ALA:HB2	1:C:487:LEU:HG	1.93	0.50
1:A:394:TRP:C	1:A:398:ARG:HD2	2.31	0.50
1:A:395:LEU:N	1:A:398:ARG:HD2	2.25	0.49
1:B:356:GLU:OE2	1:B:379:LEU:HG	2.12	0.49
1:C:34:VAL:HG11	1:C:56:LEU:HD11	1.94	0.49
1:C:120:ILE:HG22	1:C:121:LEU:H	1.77	0.49
1:C:241:HIS:O	1:C:243:GLU:N	2.33	0.49
1:A:44:VAL:HA	1:A:67:PRO:HA	1.93	0.49
1:A:391:LEU:HD23	1:A:391:LEU:O	2.13	0.49
1:A:427:MET:HB3	1:A:441:TRP:HB2	1.94	0.49
1:A:401:GLU:CD	1:A:501:ARG:HH21	2.16	0.49
1:B:464:GLN:N	1:B:466:GLY:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:HA	1:C:95:LEU:HD12	1.93	0.49
1:C:173:ARG:HG3	1:C:192:ARG:HB3	1.93	0.49
1:B:427:MET:HE2	1:B:494:VAL:HG12	1.94	0.49
1:A:341:ARG:HE	1:A:355:GLN:HE22	1.61	0.49
1:B:398:ARG:O	1:B:399:THR:HG22	2.13	0.49
1:C:222:LEU:HB2	1:C:306:GLU:OE1	2.12	0.49
1:C:163:GLN:O	1:C:167:GLY:N	2.46	0.48
1:C:407:ASP:HB2	1:C:486:CYS:HB3	1.94	0.48
1:C:489:TRP:HE3	1:C:494:VAL:HG13	1.77	0.48
1:A:464:GLN:N	1:A:466:GLY:H	2.06	0.48
1:B:173:ARG:NH2	1:B:196:ALA:HB1	2.28	0.48
1:C:95:LEU:HD12	1:C:95:LEU:H	1.78	0.48
2:A:601:BLR:NB	2:A:601:BLR:H4	2.29	0.48
1:C:261:GLU:HB3	1:C:470:HIS:CE1	2.48	0.48
1:B:458:LYS:CE	1:B:461:GLU:HG2	2.39	0.48
1:C:175:ILE:HD11	1:C:188:ILE:H	1.78	0.48
1:C:177:TYR:CE1	2:C:601:BLR:H17	2.48	0.48
1:A:464:GLN:N	1:A:465:GLY:HA2	2.28	0.48
1:C:64:LEU:HB3	1:C:238:LEU:HG	1.96	0.48
1:B:396:GLY:C	1:B:435:ARG:HH21	2.16	0.48
1:C:245:LEU:HD12	1:C:245:LEU:HA	1.48	0.48
1:A:368:ALA:HB3	1:A:379:LEU:HB2	1.94	0.48
1:C:359:LEU:HB3	1:C:362:LEU:HD23	1.96	0.48
1:A:236:ARG:HA	1:A:236:ARG:HD2	1.65	0.48
1:C:180:ASP:OD1	1:C:184:ASN:N	2.47	0.47
1:C:277:MET:O	1:C:278:LYS:HG2	2.14	0.47
1:A:363:VAL:CG1	1:A:427:MET:HE1	2.43	0.47
1:B:74:PRO:HA	1:B:77:ARG:HG3	1.96	0.47
1:C:335:HIS:HE1	1:C:499:GLU:C	2.17	0.47
1:C:479:LYS:HG3	1:C:481:THR:HG23	1.97	0.47
1:B:340:GLU:O	1:B:344:ARG:HG3	2.14	0.47
1:B:385:ASP:H	1:B:388:LEU:HB2	1.79	0.47
1:C:322:ASN:HA	1:C:324:ASP:HB2	1.96	0.47
1:A:431:MET:HB2	1:A:437:ASN:HB2	1.97	0.47
1:C:304:ALA:HA	1:C:307:PHE:HB3	1.96	0.47
1:B:37:VAL:HG12	1:B:120:ILE:HG12	1.96	0.47
1:B:407:ASP:C	1:B:422:VAL:HG11	2.35	0.47
1:C:33:GLY:HA3	1:C:252:LEU:CD1	2.45	0.47
1:C:178:ARG:HD2	1:C:179:PHE:H	1.78	0.47
1:A:397:SER:HA	1:A:398:ARG:O	2.14	0.47
1:A:427:MET:HG2	1:A:441:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:ND2	1:B:472:ARG:O	2.48	0.47
1:C:408:ARG:CZ	1:C:484:GLY:HA3	2.45	0.47
1:A:420:GLN:O	1:A:445:GLU:HB2	2.15	0.47
1:C:166:ARG:HA	1:C:169:THR:OG1	2.15	0.47
1:B:227:THR:HB	1:B:294:THR:HG22	1.96	0.46
1:C:37:VAL:HG21	1:C:47:HIS:ND1	2.31	0.46
1:C:286:ILE:HD11	1:C:312:MET:CE	2.45	0.46
1:C:461:GLU:O	1:C:463:ASP:N	2.48	0.46
1:A:166:ARG:NH1	1:A:171:PHE:O	2.48	0.46
1:A:328:ARG:NH2	1:A:495:GLU:OE1	2.45	0.46
1:B:460:VAL:HG22	2:B:601:BLR:CMC	2.45	0.46
1:A:177:TYR:CE1	1:A:185:GLY:HA3	2.50	0.46
1:C:348:PHE:HZ	1:C:505:ILE:HD11	1.81	0.46
1:C:359:LEU:HD12	1:C:441:TRP:HE1	1.81	0.46
1:C:169:THR:OG1	1:C:170:GLY:N	2.47	0.46
1:C:446:ALA:HB3	1:C:485:ARG:O	2.16	0.46
1:A:177:TYR:OH	1:A:185:GLY:HA3	2.15	0.46
1:A:211:ARG:HE	1:A:214:ARG:NH2	2.14	0.46
1:C:275:SER:CB	1:C:282:LEU:HD21	2.45	0.46
1:C:439:VAL:HG13	1:C:439:VAL:O	2.16	0.46
1:A:119:LEU:HD12	1:A:120:ILE:N	2.31	0.46
1:A:225:ILE:HD11	1:A:255:VAL:HG11	1.97	0.46
1:A:235:VAL:HG11	1:A:245:LEU:HD23	1.98	0.46
1:C:321:GLY:H	1:C:492:TYR:HE2	1.64	0.46
1:A:408:ARG:HH12	1:A:485:ARG:HH21	1.62	0.46
1:C:312:MET:C	1:C:314:SER:H	2.19	0.46
1:C:350:SER:OG	1:C:375:ARG:NH2	2.48	0.46
1:C:487:LEU:HB2	1:C:489:TRP:HD1	1.79	0.46
1:B:408:ARG:NH1	1:B:484:GLY:HA3	2.31	0.46
1:B:492:TYR:C	1:B:495:GLU:OE2	2.53	0.46
1:C:312:MET:H	1:C:312:MET:HG3	1.44	0.46
1:C:471:PRO:HB2	1:C:472:ARG:H	1.53	0.45
1:A:499:GLU:OE1	1:A:502:ARG:NH1	2.50	0.45
1:B:250:SER:HB2	1:B:253:ARG:HB2	1.96	0.45
1:B:413:TYR:HE2	1:B:419:PHE:CZ	2.34	0.45
1:B:423:ALA:O	1:B:444:PRO:HA	2.16	0.45
1:C:51:ASN:N	1:C:51:ASN:OD1	2.47	0.45
1:C:120:ILE:HG22	1:C:121:LEU:N	2.31	0.45
1:C:222:LEU:HD12	1:C:273:SER:O	2.17	0.45
1:A:77:ARG:O	1:A:81:GLU:HG2	2.15	0.45
1:C:31:PRO:HD3	1:C:230:TYR:CD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HE2	1:A:489:TRP:CZ3	2.52	0.45
1:B:363:VAL:HG21	1:B:427:MET:SD	2.57	0.45
1:C:90:LYS:HD2	1:C:90:LYS:H	1.82	0.45
1:C:322:ASN:O	1:C:323:GLU:HB2	2.17	0.45
1:B:148:LEU:CD2	1:B:161:VAL:HG23	2.43	0.45
1:B:408:ARG:O	1:B:411:ARG:HB3	2.17	0.45
1:B:422:VAL:C	1:B:424:ALA:N	2.70	0.45
1:C:155:GLN:HA	1:C:158:CYS:HB2	1.98	0.45
1:A:175:ILE:HG22	1:A:190:GLU:HA	1.98	0.45
1:A:28:ALA:HB1	1:A:232:PRO:HB2	1.98	0.45
1:B:340:GLU:O	1:B:343:ALA:HB3	2.17	0.45
1:C:304:ALA:O	1:C:307:PHE:HB3	2.17	0.45
1:A:208:ASP:OD1	1:A:208:ASP:N	2.49	0.45
1:A:455:ASN:HD22	1:A:458:LYS:HG3	1.79	0.45
1:B:247:LEU:O	1:B:253:ARG:HD3	2.16	0.45
1:A:192:ARG:NH2	1:C:81:GLU:OE2	2.50	0.44
1:B:491:ALA:O	1:B:494:VAL:HG22	2.17	0.44
1:C:203:HIS:O	1:C:452:TRP:HA	2.16	0.44
1:C:266:MET:HB3	1:C:268:VAL:HG23	2.00	0.44
1:C:268:VAL:HG13	1:C:289:HIS:HB3	1.98	0.44
1:C:276:LEU:HD11	1:C:313:SER:HA	1.98	0.44
1:C:328:ARG:NH2	1:C:496:ALA:HA	2.32	0.44
1:B:425:GLY:O	1:B:442:PHE:HA	2.17	0.44
1:C:211:ARG:NH2	1:C:215:GLU:OE2	2.50	0.44
2:A:601:BLR:H4	2:A:601:BLR:C1B	2.48	0.44
1:B:491:ALA:C	1:B:495:GLU:OE2	2.54	0.44
1:C:202:LEU:HD12	1:C:451:ASN:HB2	1.99	0.44
1:A:44:VAL:CA	1:A:67:PRO:HA	2.48	0.44
1:B:423:ALA:HB2	1:B:445:GLU:CB	2.47	0.44
1:C:209:ILE:O	1:C:214:ARG:HD3	2.17	0.44
2:C:601:BLR:NB	2:C:601:BLR:H4	2.33	0.44
1:A:398:ARG:HG3	1:A:399:THR:N	2.32	0.44
1:C:255:VAL:HG13	1:C:260:LEU:HD11	1.99	0.44
1:A:17:ASN:HA	1:A:20:ARG:CZ	2.48	0.44
1:B:388:LEU:HD23	1:B:392:ILE:HG12	1.98	0.44
1:C:158:CYS:HB3	1:C:189:ALA:CB	2.48	0.44
1:A:40:GLU:HA	1:A:42:GLY:N	2.33	0.44
1:B:29:ILE:HD11	1:B:49:SER:OG	2.17	0.44
1:C:332:LYS:HD2	1:C:336:ALA:HB2	1.99	0.44
1:A:358:GLY:O	1:A:360:LEU:N	2.49	0.44
1:A:363:VAL:HB	1:A:427:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:H	1:B:95:LEU:HG	1.62	0.44
1:A:258:ILE:HG13	1:A:471:PRO:HD3	1.99	0.44
1:A:464:GLN:HB2	1:A:466:GLY:N	2.33	0.44
1:B:374:GLY:HA3	1:B:375:ARG:CB	2.48	0.44
1:C:327:GLN:HB2	1:C:492:TYR:HD1	1.83	0.44
1:C:388:LEU:O	1:C:388:LEU:HD13	2.18	0.44
1:A:78:GLU:N	1:A:79:PRO:HD2	2.33	0.43
1:A:299:TYR:O	1:A:303:THR:HG23	2.18	0.43
1:B:341:ARG:HG3	1:B:355:GLN:HG3	2.00	0.43
1:C:27:GLY:O	1:C:234:ARG:HD3	2.16	0.43
1:C:295:ARG:O	1:C:296:TYR:HB2	2.18	0.43
1:B:39:SER:OG	1:B:44:VAL:HB	2.18	0.43
1:B:367:GLY:HA2	1:B:380:GLY:HA3	2.00	0.43
1:C:19:ASP:HA	1:C:212:GLN:CG	2.46	0.43
1:C:111:ILE:HD12	1:C:299:TYR:CZ	2.53	0.43
1:C:276:LEU:HG	1:C:312:MET:HE1	2.01	0.43
1:C:329:ILE:O	1:C:332:LYS:HG2	2.18	0.43
1:A:316:LEU:HA	1:A:316:LEU:HD23	1.53	0.43
1:A:452:TRP:CD2	1:A:456:PRO:HG3	2.53	0.43
1:C:128:HIS:O	1:C:128:HIS:ND1	2.51	0.43
1:C:217:TYR:OH	2:C:601:BLR:O1D	2.27	0.43
1:C:440:LEU:O	1:C:441:TRP:HB2	2.17	0.43
1:A:389:THR:O	1:A:392:ILE:HG22	2.18	0.43
1:A:406:THR:O	1:A:489:TRP:NE1	2.42	0.43
1:B:407:ASP:OD1	1:B:407:ASP:N	2.47	0.43
1:B:460:VAL:HG22	2:B:601:BLR:H21	2.00	0.43
1:C:278:LYS:HG3	1:C:316:LEU:CD1	2.48	0.43
1:C:497:ALA:HA	1:C:500:LEU:HB3	2.01	0.43
1:A:235:VAL:HG11	1:A:245:LEU:CD2	2.49	0.43
1:C:301:VAL:O	1:C:305:CYS:N	2.48	0.43
1:C:506:ASP:OD1	1:C:507:VAL:HG13	2.18	0.43
1:B:227:THR:HB	1:B:294:THR:CG2	2.49	0.43
1:C:325:TYR:O	1:C:326:ASP:HB2	2.19	0.43
1:C:422:VAL:HG21	1:C:486:CYS:HB2	1.99	0.43
1:C:436:ASN:HA	1:C:437:ASN:HA	1.83	0.43
1:C:436:ASN:HB3	1:C:437:ASN:OD1	2.18	0.43
1:B:362:LEU:HD11	1:B:496:ALA:HB1	1.99	0.43
1:B:374:GLY:HA3	1:B:375:ARG:CG	2.43	0.43
1:C:230:TYR:CE2	1:C:260:LEU:HD21	2.54	0.43
1:A:197:ASP:OD1	1:C:77:ARG:NH2	2.45	0.43
1:A:426:LEU:HD11	1:A:440:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:HD3	1:B:375:ARG:HA	1.81	0.43
1:C:431:MET:HE3	1:C:437:ASN:H	1.84	0.43
1:C:471:PRO:CB	2:C:601:BLR:H22	2.47	0.43
1:A:253:ARG:NH1	2:A:601:BLR:O1D	2.48	0.42
1:A:363:VAL:HB	1:A:427:MET:HE1	2.01	0.42
1:A:394:TRP:CD1	1:A:398:ARG:NE	2.87	0.42
1:B:47:HIS:CD2	1:B:237:ALA:HB2	2.54	0.42
1:B:148:LEU:HD22	1:B:157:LEU:HD12	2.01	0.42
1:A:47:HIS:CD2	1:A:245:LEU:HD22	2.54	0.42
1:B:243:GLU:H	1:B:243:GLU:HG2	1.55	0.42
1:B:378:VAL:HG12	1:B:379:LEU:H	1.85	0.42
1:C:145:LEU:HG	1:C:146:SER:N	2.33	0.42
1:C:187:VAL:CG1	1:C:200:LEU:HA	2.49	0.42
1:C:281:LYS:O	1:C:283:TRP:N	2.52	0.42
1:A:101:VAL:HG11	1:A:106:ARG:NH2	2.34	0.42
1:B:143:ASP:O	1:B:144:GLY:C	2.58	0.42
1:B:162:VAL:CG1	1:B:176:ILE:HG12	2.49	0.42
1:C:140:ALA:O	1:C:144:GLY:N	2.48	0.42
1:C:258:ILE:HG21	1:C:469:LEU:HB2	2.02	0.42
1:C:309:GLY:HA2	1:C:312:MET:SD	2.60	0.42
1:B:132:VAL:HG23	1:B:132:VAL:O	2.20	0.42
1:C:33:GLY:O	1:C:51:ASN:ND2	2.52	0.42
1:C:187:VAL:HG12	1:C:200:LEU:HA	2.00	0.42
1:C:408:ARG:CG	1:C:417:GLN:HE22	2.33	0.42
1:C:450:VAL:HG13	1:C:480:GLU:HG2	2.02	0.42
1:A:148:LEU:HD12	1:A:311:VAL:CG1	2.49	0.42
1:C:148:LEU:HD21	1:C:161:VAL:CG1	2.50	0.42
1:C:348:PHE:CZ	1:C:505:ILE:HD11	2.54	0.42
1:A:162:VAL:HG13	1:A:176:ILE:HG12	2.02	0.42
1:A:353:ALA:HA	1:A:379:LEU:HD11	2.01	0.42
1:A:363:VAL:HG11	1:A:427:MET:HE1	1.99	0.42
1:C:192:ARG:CZ	1:C:198:PRO:HB3	2.49	0.42
1:A:44:VAL:H	1:A:67:PRO:CA	2.28	0.42
1:B:124:GLU:CD	1:B:302:ARG:HH22	2.23	0.42
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.89	0.42
1:C:158:CYS:O	1:C:162:VAL:HG22	2.20	0.42
1:C:162:VAL:HG23	1:C:191:ALA:HB2	2.02	0.42
1:C:379:LEU:HD22	1:C:379:LEU:HA	1.91	0.42
1:A:506:ASP:CG	1:B:502:ARG:HH22	2.23	0.42
1:B:40:GLU:OE2	1:B:114:ARG:NE	2.52	0.42
1:C:31:PRO:HG3	1:C:231:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD23	1:C:36:LEU:N	2.35	0.42
1:C:340:GLU:HA	1:C:344:ARG:HB2	2.01	0.42
1:C:420:GLN:HG2	1:C:423:ALA:HB3	2.02	0.42
1:C:186:SER:OG	1:C:187:VAL:N	2.53	0.42
1:A:363:VAL:CG1	1:A:427:MET:CE	2.98	0.41
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.85	0.41
1:C:37:VAL:HG22	1:C:47:HIS:CB	2.49	0.41
1:C:154:LEU:HG	1:C:155:GLN:CD	2.40	0.41
1:A:290:GLN:HG2	1:A:294:THR:O	2.21	0.41
1:C:95:LEU:O	1:C:97:VAL:HG23	2.20	0.41
1:C:408:ARG:NH2	1:C:484:GLY:HA3	2.35	0.41
1:C:408:ARG:HG3	1:C:417:GLN:HE22	1.84	0.41
1:A:313:SER:HA	1:A:316:LEU:HG	2.01	0.41
1:A:400:GLY:HA2	1:A:435:ARG:HH11	1.84	0.41
1:B:443:ARG:NH2	1:B:493:GLU:OE1	2.53	0.41
1:C:165:VAL:O	1:C:169:THR:OG1	2.26	0.41
1:C:321:GLY:N	1:C:492:TYR:HE2	2.17	0.41
1:C:327:GLN:CD	1:C:490:LYS:HB2	2.40	0.41
1:C:19:ASP:HB3	1:C:212:GLN:NE2	2.34	0.41
1:C:259:HIS:CE1	2:C:601:BLR:C1A	3.03	0.41
1:C:486:CYS:SG	1:C:487:LEU:N	2.94	0.41
1:A:147:ARG:NH1	1:A:164:GLU:OE1	2.48	0.41
1:C:173:ARG:NH2	1:C:199:TYR:CZ	2.89	0.41
1:C:325:TYR:CD1	1:C:325:TYR:N	2.87	0.41
1:A:50:GLU:C	1:A:52:ALA:H	2.23	0.41
1:A:180:ASP:OD2	1:A:184:ASN:HB2	2.21	0.41
1:A:273:SER:HA	1:A:286:ILE:O	2.20	0.41
1:B:43:LEU:CD1	1:B:81:GLU:HG2	2.48	0.41
1:B:349:VAL:HG21	1:B:372:PHE:CD1	2.56	0.41
1:B:403:VAL:HG23	1:B:403:VAL:O	2.21	0.41
1:C:37:VAL:HG22	1:C:47:HIS:H	1.86	0.41
1:C:221:TRP:HE3	1:C:306:GLU:OE2	2.03	0.41
1:C:276:LEU:N	1:C:284:GLY:O	2.43	0.41
1:C:157:LEU:O	1:C:158:CYS:C	2.57	0.41
1:C:335:HIS:CE1	1:C:499:GLU:HB3	2.55	0.41
1:B:356:GLU:HB2	1:B:379:LEU:HD11	2.03	0.41
1:A:57:GLY:HA3	1:A:101:VAL:HG21	2.03	0.41
1:B:154:LEU:HA	1:B:154:LEU:HD12	1.83	0.41
1:B:423:ALA:HA	1:B:445:GLU:N	2.35	0.41
1:B:450:VAL:HG13	1:B:452:TRP:NE1	2.35	0.41
1:C:24:HIS:ND1	1:C:24:HIS:N	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:HIS:CD2	1:C:245:LEU:HD22	2.56	0.41
1:C:115:HIS:NE2	1:C:246:ASP:OD2	2.53	0.41
1:C:180:ASP:OD2	1:C:184:ASN:HB2	2.21	0.41
1:C:327:GLN:HE22	1:C:493:GLU:HB2	1.84	0.41
1:C:453:SER:OG	1:C:454:GLY:N	2.54	0.41
1:C:18:CYS:SG	1:C:210:PRO:HB3	2.62	0.41
1:C:112:ALA:HB2	1:C:121:LEU:HD13	2.03	0.41
1:C:205:PRO:HB2	1:C:207:SER:HB3	2.03	0.41
1:A:176:ILE:CD1	1:A:286:ILE:HG12	2.50	0.40
1:A:300:GLU:OE2	1:B:142:ARG:NH2	2.54	0.40
1:C:71:PHE:O	1:C:72:ILE:HB	2.21	0.40
1:C:359:LEU:HB2	1:C:441:TRP:CE2	2.56	0.40
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.83	0.40
1:B:34:VAL:HG21	1:B:56:LEU:HG	2.03	0.40
1:B:183:TRP:O	1:B:206:ALA:HA	2.21	0.40
1:B:387:ALA:HB1	1:B:419:PHE:CE1	2.56	0.40
1:B:420:GLN:NE2	1:B:423:ALA:HB1	2.35	0.40
1:C:179:PHE:HD1	1:C:183:TRP:O	2.04	0.40
1:C:316:LEU:O	1:C:320:GLU:HG3	2.21	0.40
1:A:157:LEU:O	1:A:161:VAL:HG23	2.21	0.40
1:A:449:THR:OG1	1:A:479:LYS:HD3	2.21	0.40
1:A:515:LEU:HA	1:A:515:LEU:HD12	1.77	0.40
1:B:45:LEU:HD12	1:B:45:LEU:H	1.86	0.40
1:A:455:ASN:HA	1:A:456:PRO:HD2	1.99	0.40
1:C:192:ARG:NH2	1:C:194:ALA:HA	2.36	0.40
1:C:273:SER:HA	1:C:286:ILE:O	2.21	0.40
1:C:275:SER:HA	1:C:285:LEU:HD23	2.03	0.40
1:C:301:VAL:O	1:C:304:ALA:N	2.54	0.40
1:A:205:PRO:C	1:A:207:SER:H	2.24	0.40
1:A:269:GLN:HB3	1:A:293:GLY:O	2.21	0.40
1:A:395:LEU:HA	1:A:398:ARG:HH11	1.86	0.40
1:C:153:ASP:HB3	1:C:323:GLU:OE2	2.21	0.40
1:C:220:ASN:OD1	1:C:221:TRP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	503/515 (98%)	421 (84%)	67 (13%)	15 (3%)	4 24
1	B	503/515 (98%)	426 (85%)	55 (11%)	22 (4%)	2 16
1	C	498/515 (97%)	336 (68%)	103 (21%)	59 (12%)	0 1
All	All	1504/1545 (97%)	1183 (79%)	225 (15%)	96 (6%)	1 9

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	THR
1	B	324	ASP
1	B	328	ARG
1	B	375	ARG
1	B	398	ARG
1	B	463	ASP
1	C	72	ILE
1	C	94	PRO
1	C	102	ASP
1	C	283	TRP
1	C	296	TYR
1	C	322	ASN
1	C	323	GLU
1	C	414	PRO
1	C	440	LEU
1	C	447	VAL
1	C	460	VAL
1	C	462	PHE
1	C	481	THR
1	A	14	ASP
1	A	44	VAL
1	A	128	HIS
1	A	463	ASP
1	A	484	GLY

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Mol	Chain	Res	Type
1	B	14	ASP
1	B	194	ALA
1	C	207	SER
1	C	242	GLY
1	C	282	LEU
1	C	335	HIS
1	C	358	GLY
1	C	392	ILE
1	C	421	GLU
1	C	433	ARG
1	C	506	ASP
1	A	359	LEU
1	A	448	GLN
1	A	458	LYS
1	B	327	GLN
1	B	399	THR
1	B	400	GLY
1	B	421	GLU
1	B	464	GLN
1	C	19	ASP
1	C	131	ALA
1	C	145	LEU
1	C	169	THR
1	C	303	THR
1	C	364	HIS
1	C	428	ALA
1	C	452	TRP
1	C	456	PRO
1	C	471	PRO
1	A	398	ARG
1	A	400	GLY
1	B	54	ALA
1	B	323	GLU
1	B	385	ASP
1	B	408	ARG
1	B	419	PHE
1	B	448	GLN
1	C	90	LYS
1	C	93	ASN
1	C	174	ALA
1	C	189	ALA
1	C	278	LYS

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Mol	Chain	Res	Type
1	C	378	VAL
1	C	410	ALA
1	C	419	PHE
1	A	411	ARG
1	A	455	ASN
1	B	186	SER
1	C	247	LEU
1	C	328	ARG
1	C	376	THR
1	C	379	LEU
1	C	409	LEU
1	C	412	GLU
1	C	431	MET
1	C	444	PRO
1	C	467	PRO
1	A	384	SER
1	B	131	ALA
1	C	399	THR
1	C	436	ASN
1	C	439	VAL
1	C	55	VAL
1	B	383	PRO
1	C	329	ILE
1	C	73	GLU
1	C	383	PRO
1	B	444	PRO
1	C	465	GLY
1	C	470	HIS
1	C	382	ALA
1	A	41	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	419/427 (98%)	404 (96%)	15 (4%)	35 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	419/427 (98%)	411 (98%)	8 (2%)	57 80
1	C	414/427 (97%)	392 (95%)	22 (5%)	22 55
All	All	1252/1281 (98%)	1207 (96%)	45 (4%)	35 67

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	20	ARG
1	A	39	SER
1	A	58	ASN
1	A	80	LEU
1	A	155	GLN
1	A	195	ARG
1	A	211	ARG
1	A	344	ARG
1	A	356	GLU
1	A	375	ARG
1	A	385	ASP
1	A	394	TRP
1	A	430	SER
1	A	436	ASN
1	B	88	ARG
1	B	271	SER
1	B	325	TYR
1	B	379	LEU
1	B	401	GLU
1	B	441	TRP
1	B	464	GLN
1	B	502	ARG
1	C	24	HIS
1	C	73	GLU
1	C	85	ARG
1	C	105	ASP
1	C	107	PHE
1	C	138	PHE
1	C	142	ARG
1	C	171	PHE
1	C	195	ARG
1	C	211	ARG
1	C	278	LYS

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Mol	Chain	Res	Type
1	C	295	ARG
1	C	310	GLU
1	C	312	MET
1	C	326	ASP
1	C	344	ARG
1	C	408	ARG
1	C	411	ARG
1	C	420	GLN
1	C	452	TRP
1	C	464	GLN
1	C	479	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	GLN
1	C	327	GLN
1	C	335	HIS
1	C	417	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	40,46,46	5.17	15 (37%)	44,67,67	1.97	6 (13%)
2	BLR	A	601	1	40,46,46	5.21	17 (42%)	44,67,67	1.67	10 (22%)
2	BLR	C	601	1	40,46,46	5.33	16 (40%)	44,67,67	1.68	7 (15%)

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	-	10/24/58/58	0/4/4/4
2	BLR	A	601	1	-	7/24/58/58	0/4/4/4
2	BLR	C	601	1	-	11/24/58/58	0/4/4/4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	BLR	CHA-C4D	-24.71	1.32	1.51
2	B	601	BLR	CHA-C4D	-24.43	1.33	1.51
2	A	601	BLR	CHA-C4D	-23.44	1.33	1.51
2	C	601	BLR	C1B-NB	10.42	1.55	1.37
2	C	601	BLR	C4C-NC	10.39	1.55	1.37
2	A	601	BLR	C3D-C4D	10.39	1.54	1.39
2	A	601	BLR	C4C-NC	10.33	1.55	1.37
2	B	601	BLR	C4C-NC	9.50	1.53	1.37
2	C	601	BLR	C3D-C4D	9.24	1.53	1.39
2	A	601	BLR	C1B-NB	9.19	1.53	1.37
2	B	601	BLR	C1B-NB	9.02	1.52	1.37
2	B	601	BLR	C3D-C4D	8.81	1.52	1.39
2	C	601	BLR	C1C-NC	8.20	1.55	1.38
2	A	601	BLR	C1C-NC	8.06	1.54	1.38
2	B	601	BLR	C1C-NC	7.96	1.54	1.38
2	A	601	BLR	C4B-NB	7.77	1.54	1.38
2	C	601	BLR	C4B-NB	7.67	1.54	1.38
2	B	601	BLR	C4B-NB	6.94	1.52	1.38
2	B	601	BLR	C4A-CHB	3.43	1.54	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BLR	C3C-C4C	3.35	1.51	1.45
2	B	601	BLR	C3D-C2D	3.34	1.47	1.37
2	C	601	BLR	CHA-C1A	3.32	1.54	1.51
2	A	601	BLR	C1D-CHD	3.23	1.53	1.41
2	B	601	BLR	C1D-CHD	3.06	1.53	1.41
2	C	601	BLR	C4A-CHB	3.04	1.52	1.41
2	A	601	BLR	OC-C1C	-3.04	1.17	1.23
2	A	601	BLR	C4A-CHB	3.03	1.52	1.41
2	B	601	BLR	OB-C4B	-3.01	1.17	1.23
2	A	601	BLR	OB-C4B	-3.00	1.17	1.23
2	A	601	BLR	C3D-C2D	2.98	1.46	1.37
2	B	601	BLR	OC-C1C	-2.88	1.18	1.23
2	C	601	BLR	C1D-CHD	2.85	1.52	1.41
2	C	601	BLR	C3D-C2D	2.78	1.45	1.37
2	A	601	BLR	C3C-C2C	2.76	1.42	1.37
2	C	601	BLR	OB-C4B	-2.74	1.18	1.23
2	B	601	BLR	CAB-C3B	2.66	1.54	1.47
2	B	601	BLR	C3C-C2C	2.56	1.42	1.37
2	C	601	BLR	C3C-C4C	2.44	1.49	1.45
2	C	601	BLR	C1B-C2B	2.42	1.49	1.45
2	B	601	BLR	CAC-C3C	2.39	1.53	1.47
2	B	601	BLR	C3C-C4C	2.36	1.49	1.45
2	C	601	BLR	C3B-C2B	2.34	1.42	1.37
2	A	601	BLR	C1B-C2B	2.32	1.49	1.45
2	A	601	BLR	CHA-C1A	2.27	1.53	1.51
2	A	601	BLR	CAC-C3C	2.25	1.53	1.47
2	C	601	BLR	OC-C1C	-2.23	1.19	1.23
2	C	601	BLR	C3C-C2C	2.15	1.41	1.37
2	A	601	BLR	CAA-C2A	2.01	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	BLR	CAD-C3D-C4D	-8.23	121.51	127.30
2	B	601	BLR	C1B-NB-C4B	-4.51	104.93	110.67
2	C	601	BLR	CBA-CAA-C2A	-4.46	105.01	112.62
2	C	601	BLR	C1B-NB-C4B	-4.44	105.02	110.67
2	B	601	BLR	CAA-C2A-C1A	4.27	130.30	127.30
2	A	601	BLR	C1B-NB-C4B	-3.92	105.68	110.67
2	B	601	BLR	C4C-NC-C1C	-3.63	106.05	110.67
2	A	601	BLR	O1D-CGD-O2D	-3.36	114.91	123.30
2	C	601	BLR	C4C-NC-C1C	-3.36	106.39	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	BLR	CBD-CAD-C3D	-3.25	107.08	112.62
2	A	601	BLR	O1D-CGD-CBD	3.24	124.43	114.03
2	A	601	BLR	CAD-C3D-C4D	-2.99	125.19	127.30
2	A	601	BLR	O1A-CGA-CBA	2.97	123.58	114.03
2	A	601	BLR	C4C-NC-C1C	-2.96	106.89	110.67
2	A	601	BLR	CBD-CAD-C3D	-2.89	107.68	112.62
2	A	601	BLR	C3B-C2B-C1B	2.47	111.02	108.03
2	B	601	BLR	OC-C1C-NC	2.40	130.66	125.08
2	A	601	BLR	CAA-C2A-C1A	2.37	128.96	127.30
2	A	601	BLR	O1A-CGA-O2A	-2.31	117.55	123.30
2	B	601	BLR	CMA-C3A-C2A	-2.24	120.72	124.94
2	C	601	BLR	CAA-C2A-C1A	-2.12	125.80	127.30
2	C	601	BLR	CHB-C1B-C2B	-2.09	122.84	126.97
2	C	601	BLR	O1A-CGA-CBA	2.06	120.66	114.03

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BLR	NA-C4A-CHB-C1B
2	A	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C2A-C1A-CHA-C4D
2	B	601	BLR	C3D-C4D-CHA-C1A
2	B	601	BLR	NA-C4A-CHB-C1B
2	B	601	BLR	C3A-C4A-CHB-C1B
2	C	601	BLR	NA-C4A-CHB-C1B
2	C	601	BLR	C3A-C4A-CHB-C1B
2	C	601	BLR	NB-C1B-CHB-C4A
2	C	601	BLR	C2B-C1B-CHB-C4A
2	C	601	BLR	C2C-C3C-CAC-CBC
2	C	601	BLR	C2A-CAA-CBA-CGA
2	B	601	BLR	C2A-CAA-CBA-CGA
2	C	601	BLR	C4C-C3C-CAC-CBC
2	A	601	BLR	NB-C1B-CHB-C4A
2	B	601	BLR	NB-C1B-CHB-C4A
2	C	601	BLR	CAD-CBD-CGD-O2D
2	A	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAD-CBD-CGD-O1D
2	C	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
2	C	601	BLR	C2A-C1A-CHA-C4D
2	B	601	BLR	CAA-CBA-CGA-O1A
2	B	601	BLR	CAA-CBA-CGA-O2A
2	A	601	BLR	CAA-CBA-CGA-O1A
2	C	601	BLR	CAA-CBA-CGA-O1A

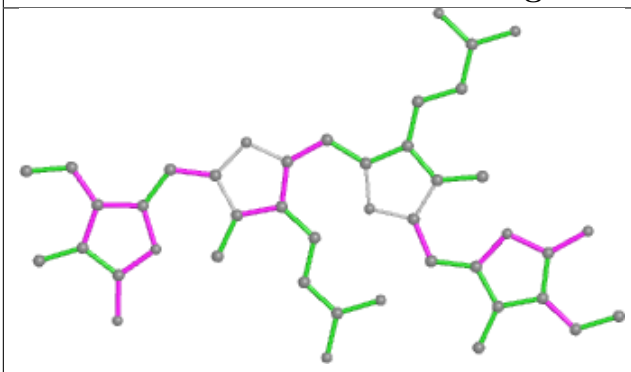
There are no ring outliers.

3 monomers are involved in 20 short contacts:

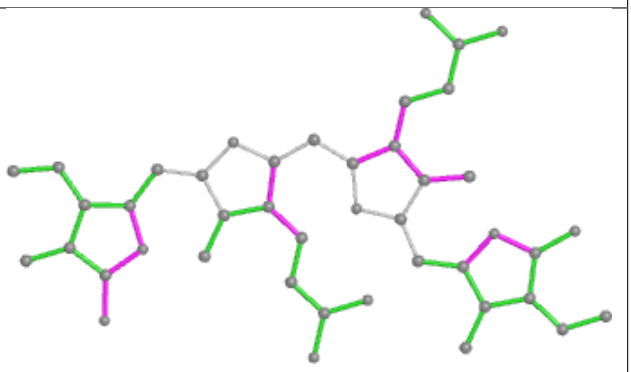
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BLR	5	0
2	A	601	BLR	5	0
2	C	601	BLR	10	0

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

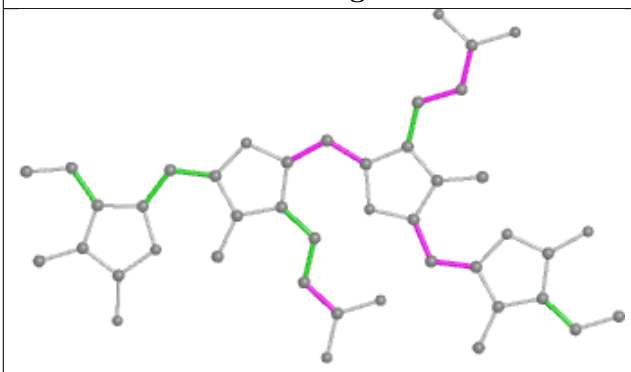
Ligand BLR B 601



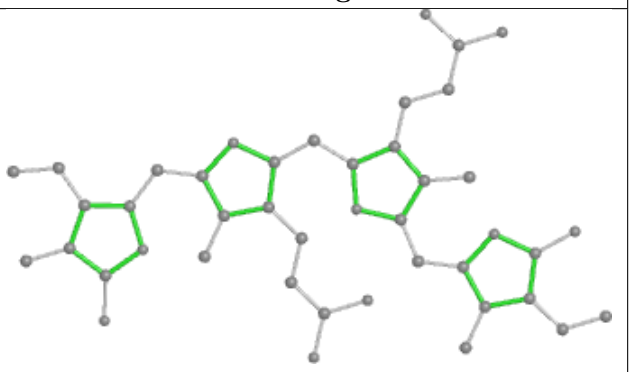
Bond lengths



Bond angles

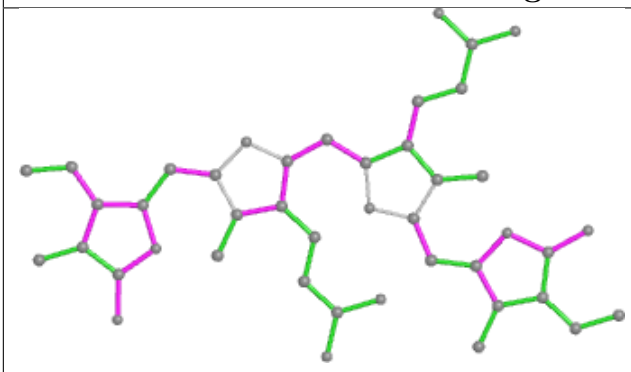


Torsions

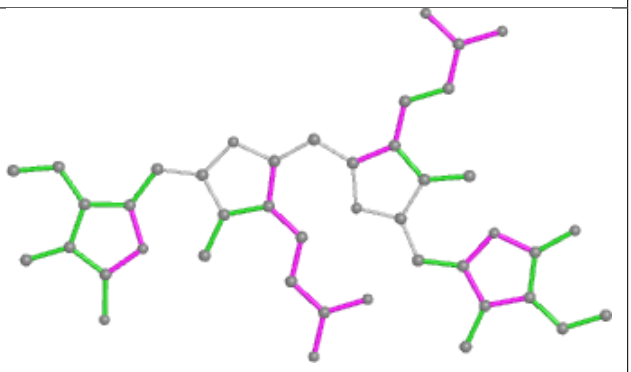


Rings

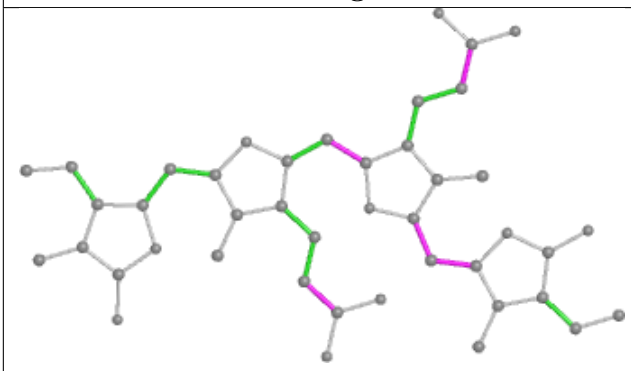
Ligand BLR A 601



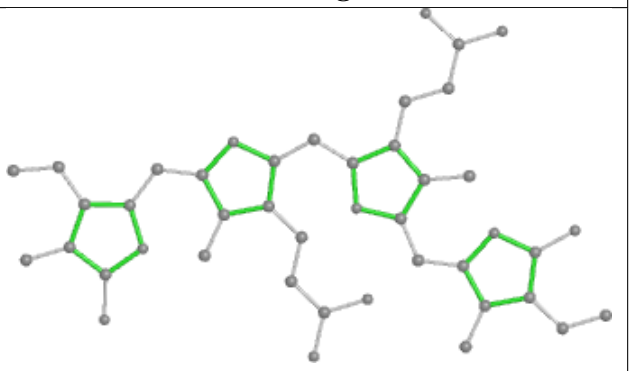
Bond lengths



Bond angles

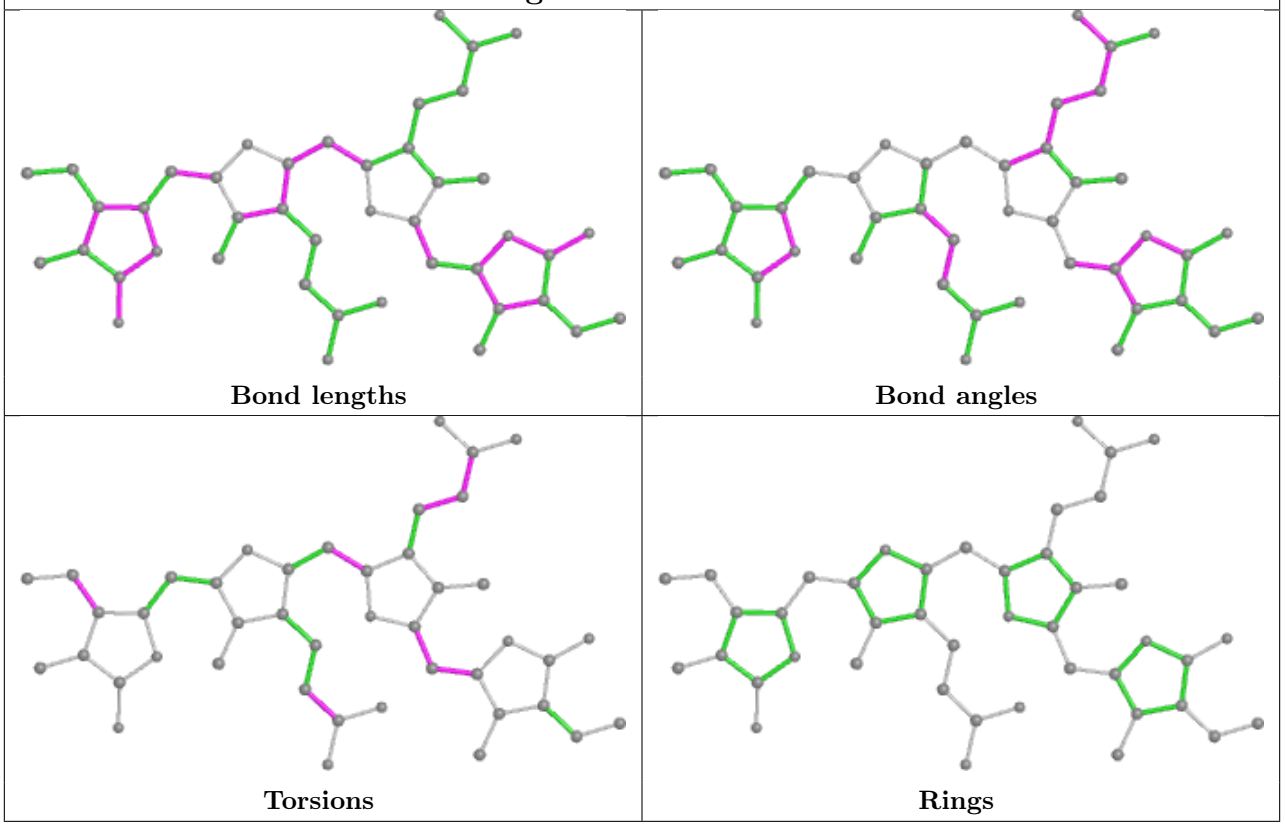


Torsions



Rings

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, 95^{th} 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%)	-0.17	12 (2%) 59 43	78, 111, 148, 229	2 (0%)
1	B	505/515 (98%)	-0.19	7 (1%) 75 63	80, 113, 165, 204	1 (0%)
1	C	500/515 (97%)	0.77	81 (16%) 1 1	102, 159, 262, 279	2 (0%)
All	All	1510/1545 (97%)	0.14	100 (6%) 18 10	78, 122, 245, 279	5 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	369	ALA	26.2
1	C	386	GLU	15.1
1	C	504	ILE	14.6
1	C	337	ALA	12.5
1	C	368	ALA	12.3
1	C	384	SER	12.1
1	C	387	ALA	11.7
1	C	499	GLU	11.2
1	C	338	LEU	11.0
1	C	405	CYS	10.8
1	C	385	ASP	10.5
1	C	339	LEU	10.0
1	C	424	ALA	9.7
1	C	440	LEU	9.6
1	A	12	GLU	8.8
1	C	374	GLY	8.5
1	C	423	ALA	8.3
1	C	373	HIS	8.2
1	C	383	PRO	8.1
1	A	14	ASP	8.0
1	A	13	VAL	7.0
1	C	441	TRP	6.4
1	C	425	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	505	ILE	5.7
1	C	370	ILE	5.6
1	C	422	VAL	5.6
1	C	488	PRO	5.5
1	C	507	VAL	5.4
1	C	342	MET	5.2
1	C	363	VAL	5.0
1	C	515	LEU	5.0
1	C	132	VAL	5.0
1	C	404	PHE	5.0
1	C	500	LEU	4.9
1	C	129	ARG	4.6
1	A	245	LEU	4.5
1	A	16	THR	4.4
1	C	496	ALA	4.4
1	C	503	SER	4.3
1	B	400	GLY	4.1
1	A	15	LEU	4.1
1	C	466	GLY	4.0
1	C	498	SER	4.0
1	C	403	VAL	3.8
1	B	398	ARG	3.8
1	C	442	PHE	3.8
1	C	297	VAL	3.7
1	C	372	PHE	3.6
1	C	457	THR	3.5
1	C	392	ILE	3.5
1	C	346	VAL	3.4
1	C	358	GLY	3.4
1	C	330	ARG	3.1
1	C	407	ASP	3.0
1	C	465	GLY	3.0
1	C	432	SER	3.0
1	C	287	SER	3.0
1	C	418	ALA	3.0
1	C	453	SER	2.9
1	C	502	ARG	2.9
1	B	13	VAL	2.9
1	C	181	ALA	2.7
1	C	413	TYR	2.7
1	C	491	ALA	2.7
1	B	12	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	376	THR	2.6
1	C	416	ALA	2.6
1	A	440	LEU	2.6
1	C	367	GLY	2.6
1	C	508	ALA	2.6
1	C	401	GLU	2.6
1	B	438	PHE	2.6
1	A	462	PHE	2.5
1	C	390	GLY	2.5
1	C	175	ILE	2.5
1	C	459	ALA	2.5
1	C	336	ALA	2.4
1	C	506	ASP	2.4
1	C	433	ARG	2.4
1	C	435	ARG	2.4
1	A	369	ALA	2.3
1	B	442	PHE	2.3
1	A	431	MET	2.3
1	C	343	ALA	2.3
1	C	325	TYR	2.3
1	B	426	LEU	2.3
1	C	443	ARG	2.2
1	C	409	LEU	2.2
1	C	439	VAL	2.2
1	A	45	LEU	2.2
1	C	402	GLY	2.1
1	C	467	PRO	2.1
1	C	371	HIS	2.1
1	C	378	VAL	2.1
1	C	334	ILE	2.1
1	C	357	SER	2.1
1	C	63	LEU	2.1
1	C	307	PHE	2.0
1	C	99	TRP	2.0
1	A	368	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

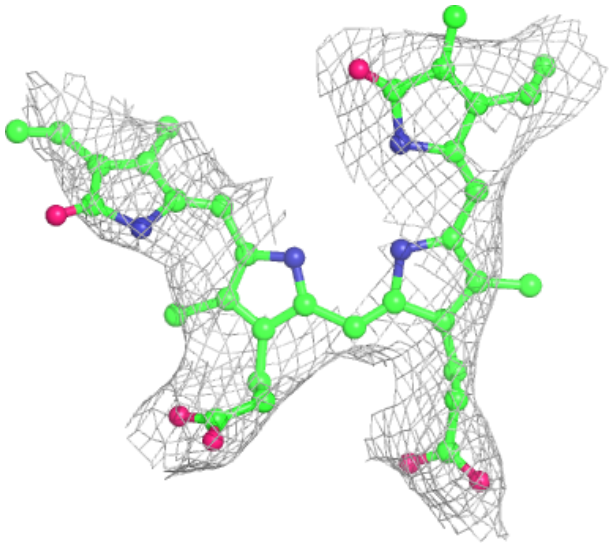
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

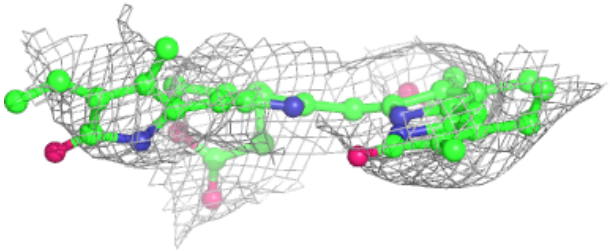
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BLR	C	601	43/43	0.92	0.28	130,146,160,163	0
2	BLR	B	601	43/43	0.93	0.27	82,94,102,112	1
2	BLR	A	601	43/43	0.94	0.46	82,104,124,127	1

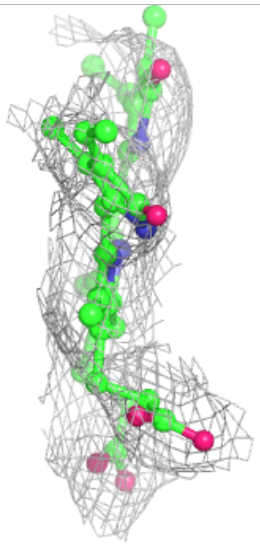
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

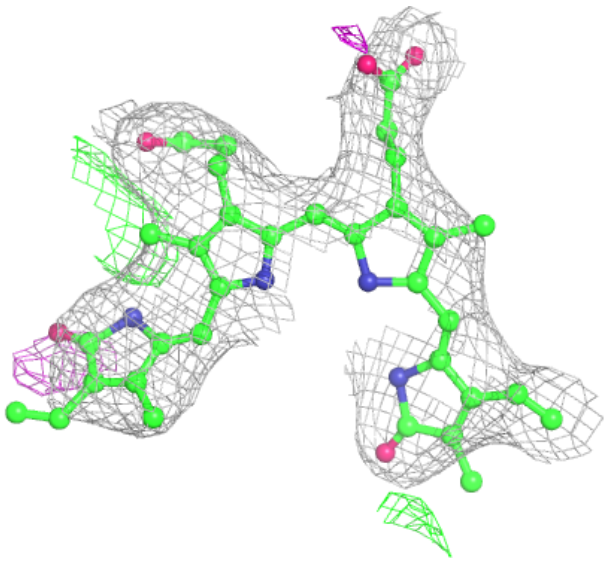


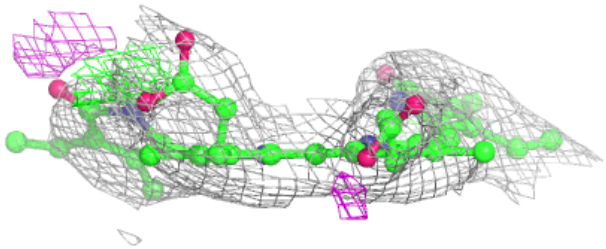


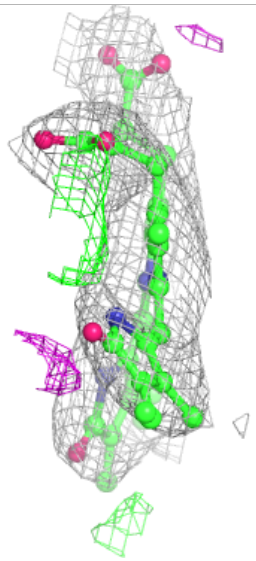


Electron density around BLR B 601:

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

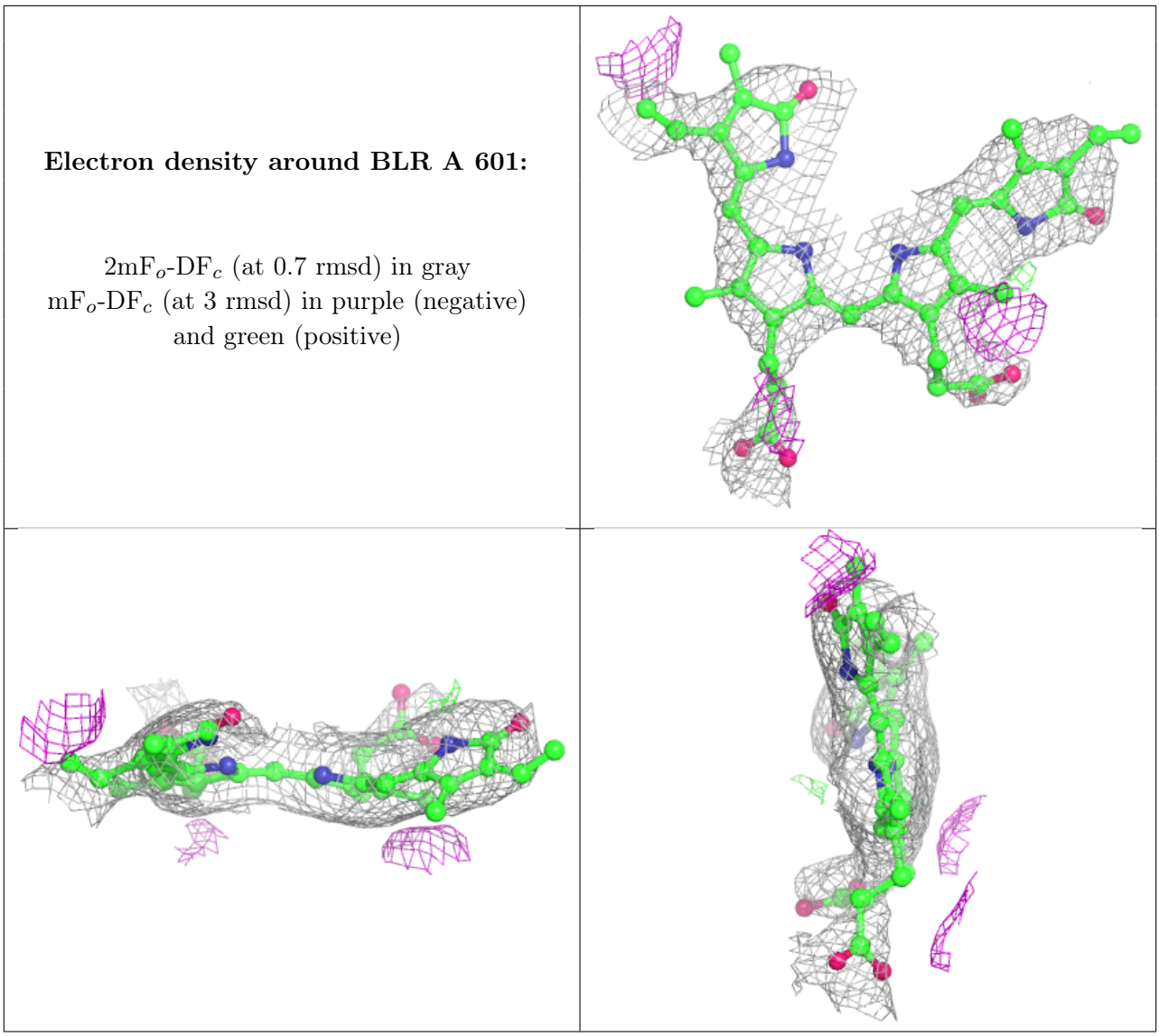






Electron density around BLR A 601:

$2mF_o$-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.