



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 02:33 pm GMT

PDB ID : 4UYM
Title : Crystal structure of sterol 14-alpha demethylase (CYP51B) from a pathogenic filamentous fungus *Aspergillus fumigatus* in complex with voriconazole
Authors : Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on : 2014-09-02
Resolution : 2.55 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

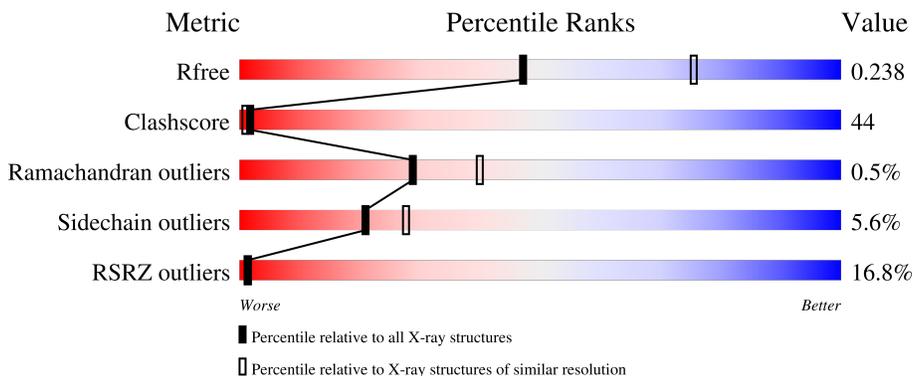
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

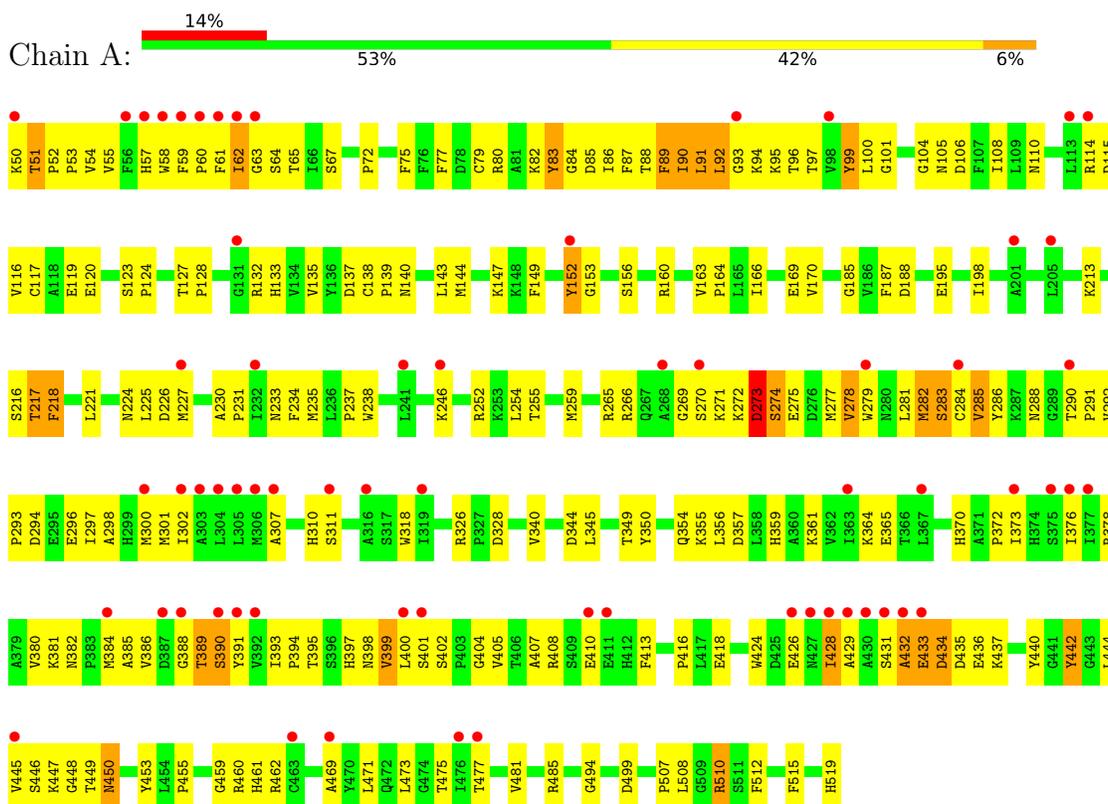
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	470	
1	B	470	

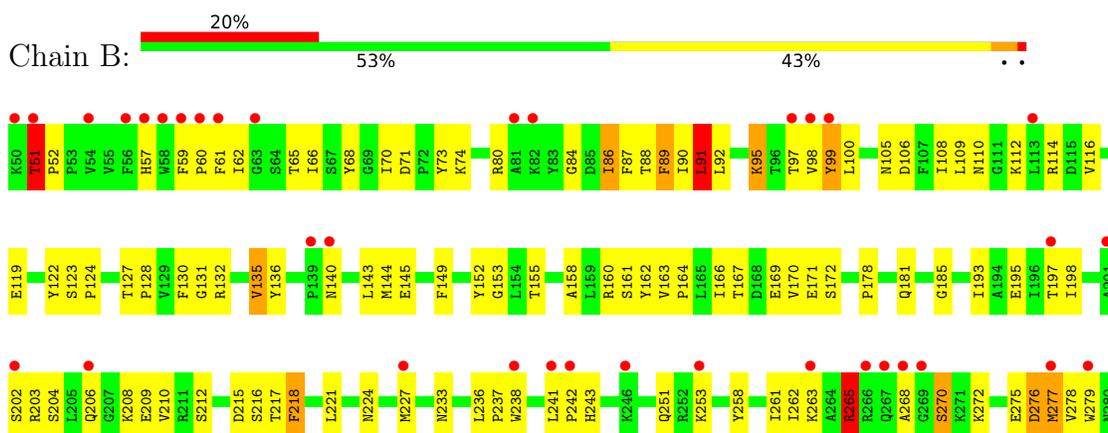
3 Residue-property plots i

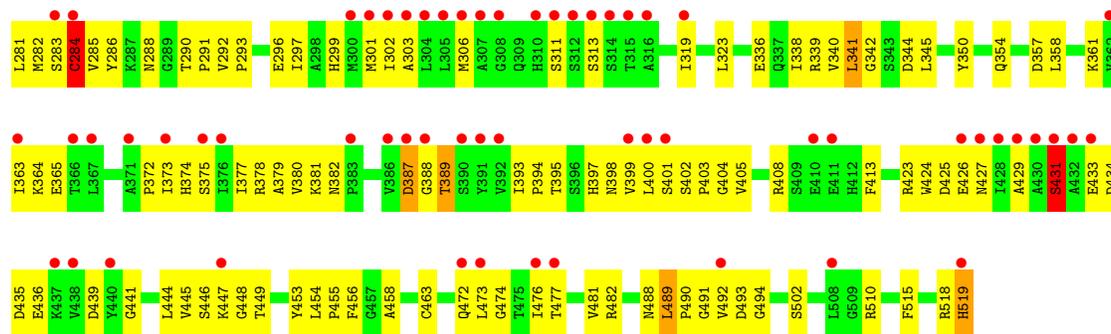
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 14-ALPHA STEROL DEMETHYLASE



• Molecule 1: 14-ALPHA STEROL DEMETHYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	109.19Å 109.19Å 90.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 28.01 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.55) 99.4 (28.01-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.210 , 0.239 0.217 , 0.238	Depositor DCC
R_{free} test set	1905 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.035 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: HEM, VOR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3854	0.62	5/5229 (0.1%)
1	B	0.35	0/3854	0.62	7/5229 (0.1%)
All	All	0.40	0/7708	0.62	12/10458 (0.1%)

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	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	B	265	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	A	217	THR	CB-CA-C	-6.00	95.41	111.60
1	A	89	PHE	N-CA-C	-5.84	95.23	111.00
1	B	89	PHE	N-CA-C	-5.47	96.24	111.00
1	B	95	LYS	N-CA-C	-5.47	96.24	111.00
1	B	284	CYS	N-CA-C	-5.44	96.32	111.00
1	B	90	ILE	CB-CA-C	-5.27	101.07	111.60
1	B	91	LEU	N-CA-C	-5.27	96.78	111.00
1	A	442	TYR	N-CA-C	-5.24	96.86	111.00
1	A	285	VAL	N-CA-C	5.17	124.97	111.00
1	A	273	ASP	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ASP	Peptide
1	A	388	GLY	Peptide
1	A	432	ALA	Peptide
1	A	485	ARG	Sidechain
1	A	93	GLY	Peptide
1	B	270	SER	Peptide
1	B	431	SER	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	3752	0	3719	357	0
1	B	3752	0	3719	290	0
2	A	43	0	30	5	0
2	B	43	0	30	8	0
3	A	25	0	14	4	0
3	B	25	0	14	6	0
4	A	87	0	0	11	0
4	B	76	0	0	12	0
All	All	7803	0	7526	660	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 44.

All (660) 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:265:ARG:NH1	1:A:277:MET:HG3	1.33	1.43
1:B:152:TYR:HB3	1:B:279:TRP:CZ2	1.69	1.25
1:B:262:ILE:HG12	1:B:277:MET:CE	1.74	1.17
1:B:224:ASN:HA	1:B:227:MET:HE2	1.18	1.15
1:A:86:ILE:HD11	1:A:99:TYR:CD1	1.81	1.15
1:B:262:ILE:HG12	1:B:277:MET:HE1	1.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:OG1	1:A:52:PRO:HD3	1.48	1.13
1:B:519:HIS:HA	4:B:2076:HOH:O	1.46	1.12
1:A:94:LYS:HE3	1:A:398:ASN:ND2	1.65	1.11
1:A:65:THR:HG22	1:A:91:LEU:HA	1.19	1.10
1:A:55:VAL:HG13	1:A:88:THR:O	1.51	1.09
1:B:106:ASP:HB2	1:B:449:THR:HG21	1.29	1.09
1:B:51:THR:HB	1:B:52:PRO:CD	1.85	1.07
1:A:284:CYS:O	1:A:292:VAL:HG23	1.56	1.06
1:A:275:GLU:HG3	1:A:277:MET:HB3	1.36	1.05
1:A:59:PHE:CD1	1:A:60:PRO:HD2	1.91	1.04
1:B:152:TYR:HB3	1:B:279:TRP:CE2	1.92	1.04
1:B:284:CYS:O	1:B:292:VAL:HG23	1.57	1.04
1:A:90:ILE:HD12	1:A:90:ILE:H	1.20	1.02
1:A:265:ARG:HH12	1:A:277:MET:HG3	1.23	1.02
1:B:493:ASP:OD1	1:B:494:GLY:N	1.92	1.02
1:A:50:LYS:O	1:A:51:THR:HG22	1.58	1.01
1:A:90:ILE:HG22	1:A:95:LYS:HA	1.38	1.01
1:B:152:TYR:HB3	1:B:279:TRP:HZ2	1.26	1.01
1:A:110:ASN:OD1	1:A:447:LYS:HB2	1.61	1.01
1:A:51:THR:OG1	1:A:52:PRO:CD	2.07	1.01
1:A:152:TYR:HB3	1:A:279:TRP:CZ2	1.97	1.00
1:A:217:THR:O	1:A:217:THR:HG22	1.62	0.99
1:A:59:PHE:CD2	1:A:62:ILE:HG12	1.98	0.99
1:A:265:ARG:NH1	1:A:277:MET:CG	2.24	0.98
1:B:106:ASP:CB	1:B:449:THR:HG21	1.93	0.98
1:A:53:PRO:HD3	1:A:391:TYR:CE1	1.98	0.98
1:B:209:GLU:N	1:B:209:GLU:OE1	1.97	0.97
1:A:55:VAL:HG21	1:A:89:PHE:CB	1.96	0.96
1:B:473:LEU:O	1:B:477:THR:HG23	1.64	0.96
1:A:65:THR:HG21	1:A:92:LEU:H	1.31	0.96
1:B:65:THR:OG1	1:B:92:LEU:HD21	1.67	0.94
1:B:95:LYS:HD3	1:B:397:HIS:NE2	1.83	0.94
1:B:106:ASP:HB2	1:B:449:THR:CG2	1.96	0.94
1:A:90:ILE:CG2	1:A:95:LYS:HA	1.98	0.94
1:B:51:THR:HB	1:B:52:PRO:HD2	1.48	0.93
1:A:51:THR:O	1:A:391:TYR:HD1	1.52	0.93
1:A:119:GLU:OE1	1:A:119:GLU:N	2.03	0.92
1:A:216:SER:O	1:A:217:THR:HB	1.69	0.92
1:B:224:ASN:CA	1:B:227:MET:HE2	1.99	0.91
1:A:59:PHE:CG	1:A:60:PRO:HD2	2.05	0.91
1:A:114:ARG:NE	1:A:115:ASP:OD1	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CB	1:B:279:TRP:HE1	1.84	0.90
1:A:361:LYS:NZ	1:A:428:ILE:HG22	1.86	0.90
1:B:224:ASN:HA	1:B:227:MET:CE	2.01	0.89
1:A:124:PRO:O	1:A:128:PRO:CD	2.21	0.89
1:A:55:VAL:CG2	1:A:89:PHE:HA	2.03	0.88
1:B:153:GLY:N	1:B:279:TRP:NE1	2.21	0.88
1:A:55:VAL:HG22	1:A:88:THR:O	1.72	0.88
1:B:265:ARG:CZ	1:B:275:GLU:OE2	2.22	0.87
1:A:413:PHE:O	1:A:416:PRO:HG3	1.73	0.87
1:A:152:TYR:HB3	1:A:279:TRP:HZ2	1.38	0.86
1:A:51:THR:O	1:A:391:TYR:CD1	2.28	0.86
1:B:152:TYR:CB	1:B:279:TRP:CZ2	2.58	0.86
1:A:55:VAL:CG1	1:A:88:THR:O	2.23	0.86
1:A:188:ASP:OD2	1:A:510:ARG:HD3	1.74	0.86
1:A:62:ILE:O	1:A:65:THR:HG23	1.75	0.86
1:A:59:PHE:CE2	1:A:62:ILE:HG23	2.11	0.85
1:A:59:PHE:HD2	1:A:62:ILE:HG12	1.37	0.85
1:A:65:THR:HG22	1:A:91:LEU:CA	2.06	0.85
1:B:95:LYS:CD	1:B:397:HIS:NE2	2.39	0.85
1:A:115:ASP:HB3	1:A:384:MET:CE	2.06	0.84
1:A:433:GLU:HG2	1:A:434:ASP:H	1.41	0.84
1:B:149:PHE:O	1:B:152:TYR:HB2	1.76	0.84
1:A:124:PRO:O	1:A:128:PRO:HD3	1.77	0.84
1:B:152:TYR:HB2	1:B:279:TRP:HE1	1.40	0.84
1:A:53:PRO:HD3	1:A:391:TYR:HE1	1.42	0.84
1:A:90:ILE:HG22	1:A:95:LYS:CA	2.07	0.84
1:A:224:ASN:HA	1:A:227:MET:HE2	1.60	0.83
1:A:92:LEU:HD12	1:A:235:MET:HE2	1.60	0.83
1:B:262:ILE:CG1	1:B:277:MET:HE1	2.08	0.83
1:B:158:ALA:O	1:B:161:SER:HB3	1.79	0.82
1:B:106:ASP:CA	1:B:449:THR:HG21	2.09	0.82
1:B:95:LYS:HD2	1:B:397:HIS:CD2	2.15	0.81
1:A:217:THR:O	1:A:217:THR:CG2	2.28	0.81
1:A:51:THR:HG23	1:A:52:PRO:N	1.96	0.81
1:A:94:LYS:HE3	1:A:398:ASN:HD21	1.44	0.81
1:A:85:ASP:O	1:A:86:ILE:HD13	1.79	0.81
1:A:361:LYS:HZ3	1:A:428:ILE:HG22	1.45	0.81
1:B:152:TYR:CB	1:B:279:TRP:NE1	2.44	0.80
1:B:210:VAL:HG13	1:B:218:PHE:CE2	2.16	0.80
1:B:262:ILE:HG12	1:B:277:MET:HE2	1.61	0.80
1:A:284:CYS:HB2	1:A:291:PRO:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HB2	1:A:83:TYR:CD1	2.18	0.79
1:A:97:THR:HG1	1:A:397:HIS:HD1	1.29	0.79
1:A:50:LYS:O	1:A:51:THR:CG2	2.30	0.79
1:B:51:THR:CB	1:B:52:PRO:CD	2.61	0.78
1:A:216:SER:O	1:A:217:THR:CB	2.32	0.78
1:B:65:THR:CB	1:B:92:LEU:HD21	2.14	0.77
1:B:66:ILE:O	1:B:70:ILE:HG12	1.85	0.77
1:A:82:LYS:HB2	1:A:83:TYR:CE1	2.20	0.77
1:A:195:GLU:O	1:A:198:ILE:HG22	1.85	0.76
1:B:152:TYR:HB3	1:B:279:TRP:NE1	2.00	0.76
1:A:59:PHE:CE1	1:A:60:PRO:HD2	2.20	0.76
1:A:65:THR:CG2	1:A:91:LEU:HA	2.08	0.76
1:A:91:LEU:HD12	1:A:91:LEU:O	1.85	0.76
1:A:326:ARG:NH2	1:A:328:ASP:OD2	2.19	0.76
1:A:275:GLU:CG	1:A:277:MET:HB3	2.16	0.75
1:B:210:VAL:HG13	1:B:218:PHE:HE2	1.51	0.75
1:A:447:LYS:HA	1:A:459:GLY:H	1.51	0.74
1:B:209:GLU:OE2	1:B:265:ARG:NH2	2.20	0.74
1:A:404:GLY:O	1:A:407:ALA:HB3	1.88	0.74
1:A:97:THR:OG1	1:A:397:HIS:ND1	2.18	0.74
1:B:444:LEU:O	1:B:445:VAL:HG13	1.87	0.74
1:A:79:CYS:HB3	1:A:87:PHE:CZ	2.22	0.74
1:A:55:VAL:HG21	1:A:89:PHE:CA	2.17	0.74
1:B:195:GLU:O	1:B:198:ILE:HG22	1.88	0.74
1:A:59:PHE:CD2	1:A:62:ILE:HG23	2.23	0.73
1:A:86:ILE:CD1	1:A:99:TYR:CD1	2.67	0.73
1:B:106:ASP:OD1	1:B:110:ASN:ND2	2.21	0.73
1:B:152:TYR:C	1:B:279:TRP:CE2	2.62	0.73
1:B:388:GLY:O	1:B:389:THR:HG23	1.87	0.73
1:A:429:ALA:HB1	1:A:431:SER:O	1.89	0.73
1:A:55:VAL:CG2	1:A:88:THR:O	2.37	0.73
1:B:152:TYR:CB	1:B:279:TRP:HZ2	1.96	0.73
1:A:266:ARG:NH2	1:A:294:ASP:OD2	2.21	0.73
1:A:432:ALA:HB1	1:A:433:GLU:HB2	1.69	0.73
1:A:86:ILE:HD11	1:A:99:TYR:CG	2.24	0.72
1:A:55:VAL:HG21	1:A:89:PHE:HB3	1.68	0.72
1:A:357:ASP:OD2	1:A:361:LYS:HE2	1.88	0.72
1:B:381:LYS:O	1:B:382:ASN:OD1	2.08	0.72
1:B:152:TYR:O	1:B:279:TRP:CZ2	2.42	0.72
1:A:90:ILE:HD12	1:A:90:ILE:N	1.99	0.72
1:B:65:THR:HB	1:B:92:LEU:CD2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:O	1:A:300:MET:HG3	1.90	0.71
1:B:98:VAL:CG1	1:B:100:LEU:HD21	2.20	0.71
1:A:361:LYS:NZ	1:A:428:ILE:CG2	2.52	0.71
1:A:435:ASP:HB2	1:A:448:GLY:HA3	1.71	0.71
1:A:55:VAL:HG21	1:A:89:PHE:HA	1.71	0.71
1:A:51:THR:CB	1:A:52:PRO:CD	2.69	0.71
1:A:365:GLU:OE1	1:A:365:GLU:HA	1.90	0.71
1:B:275:GLU:HG3	1:B:277:MET:HB3	1.71	0.71
1:A:277:MET:CE	1:A:277:MET:HA	2.21	0.70
3:B:590:VOR:C21	3:B:590:VOR:C17	2.69	0.70
1:A:86:ILE:CD1	1:A:99:TYR:HA	2.21	0.70
1:B:444:LEU:O	1:B:445:VAL:CG1	2.39	0.70
1:B:288:ASN:ND2	1:B:290:THR:OG1	2.25	0.70
1:A:255:THR:O	1:A:259:MET:HG3	1.92	0.70
1:A:277:MET:HA	1:A:277:MET:HE2	1.73	0.70
1:A:90:ILE:HG22	1:A:94:LYS:O	1.91	0.70
1:A:55:VAL:HG22	1:A:89:PHE:HA	1.73	0.70
1:B:268:ALA:HB1	4:B:2039:HOH:O	1.92	0.69
1:A:51:THR:HG23	1:A:52:PRO:CD	2.23	0.69
1:A:435:ASP:CB	1:A:448:GLY:HA3	2.22	0.69
1:B:65:THR:CB	1:B:92:LEU:CD2	2.70	0.69
1:B:463:CYS:HB2	2:B:580:HEM:NA	2.06	0.69
1:A:442:TYR:CE2	1:A:445:VAL:HG11	2.28	0.69
1:B:209:GLU:HB2	1:B:261:ILE:HD13	1.75	0.69
1:B:400:LEU:HD23	1:B:401:SER:N	2.08	0.69
1:B:265:ARG:NH2	1:B:275:GLU:OE2	2.26	0.69
1:A:114:ARG:HG3	1:A:115:ASP:OD1	1.93	0.68
1:A:94:LYS:CE	1:A:398:ASN:ND2	2.49	0.68
1:B:436:GLU:OE2	1:B:447:LYS:HE2	1.92	0.68
1:A:275:GLU:HG2	1:A:278:VAL:HG23	1.76	0.68
1:B:185:GLY:HA3	1:B:515:PHE:CE2	2.27	0.68
1:B:364:LYS:NZ	1:B:429:ALA:O	2.22	0.68
1:A:288:ASN:OD1	1:A:290:THR:N	2.26	0.68
1:B:71:ASP:OD2	1:B:74:LYS:HD3	1.94	0.67
1:B:463:CYS:HB2	2:B:580:HEM:C1A	2.29	0.67
1:A:428:ILE:C	1:A:428:ILE:HD12	2.15	0.67
1:B:132:ARG:H	1:B:299:HIS:CE1	2.11	0.67
1:B:373:ILE:HD12	1:B:373:ILE:N	2.09	0.67
3:A:590:VOR:C17	3:A:590:VOR:H21	2.23	0.67
1:B:152:TYR:C	1:B:279:TRP:NE1	2.48	0.67
1:A:284:CYS:O	1:A:292:VAL:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:VAL:HG12	1:A:286:TYR:O	1.95	0.67
1:A:58:TRP:CG	1:A:58:TRP:O	2.48	0.67
1:A:90:ILE:HG22	1:A:94:LYS:C	2.16	0.66
1:A:282:MET:C	1:A:284:CYS:H	1.98	0.66
1:A:404:GLY:O	1:A:408:ARG:HG2	1.96	0.66
1:A:288:ASN:OD1	1:A:290:THR:HG22	1.96	0.66
1:A:266:ARG:HH22	1:A:294:ASP:CG	1.99	0.66
1:A:378:ARG:HB2	1:A:399:VAL:HG23	1.78	0.66
1:B:65:THR:HB	1:B:92:LEU:HD23	1.77	0.66
1:A:94:LYS:CE	1:A:398:ASN:HD21	2.09	0.66
1:A:402:SER:OG	1:A:405:VAL:HG23	1.94	0.66
1:B:152:TYR:C	1:B:279:TRP:CZ2	2.70	0.65
1:A:394:PRO:O	1:A:397:HIS:HB2	1.97	0.65
1:A:510:ARG:HE	1:A:510:ARG:HA	1.61	0.65
1:B:152:TYR:CB	1:B:279:TRP:CE2	2.75	0.65
1:B:380:VAL:HG23	1:B:397:HIS:O	1.97	0.65
1:A:79:CYS:HB3	1:A:87:PHE:CE2	2.31	0.65
1:A:386:VAL:HG22	1:A:391:TYR:O	1.96	0.65
1:A:217:THR:O	1:A:221:LEU:HG	1.96	0.65
3:A:590:VOR:C17	3:A:590:VOR:C21	2.74	0.65
1:B:433:GLU:OE1	1:B:446:SER:OG	2.15	0.65
1:B:463:CYS:HA	2:B:580:HEM:C4D	2.32	0.65
1:B:404:GLY:O	1:B:408:ARG:HG2	1.96	0.64
1:B:340:VAL:HG23	1:B:341:LEU:HD23	1.79	0.64
1:A:55:VAL:CG2	1:A:89:PHE:CA	2.73	0.64
1:A:400:LEU:HD23	1:A:401:SER:N	2.12	0.64
1:B:286:TYR:OH	1:B:296:GLU:OE1	2.15	0.64
1:B:342:GLY:HA3	1:B:344:ASP:OD1	1.98	0.64
1:A:143:LEU:O	1:A:147:LYS:HG3	1.98	0.64
1:A:440:TYR:HE1	1:A:445:VAL:HG23	1.62	0.64
1:B:435:ASP:HB2	1:B:448:GLY:HA3	1.79	0.63
1:A:283:SER:O	1:A:283:SER:OG	2.16	0.63
1:A:266:ARG:NH1	4:A:2050:HOH:O	2.23	0.63
1:B:153:GLY:CA	1:B:279:TRP:CD1	2.82	0.63
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.98	0.63
1:B:98:VAL:HG12	1:B:100:LEU:CD2	2.29	0.63
1:A:265:ARG:HH22	1:A:275:GLU:CD	2.02	0.63
1:A:59:PHE:HE2	1:A:62:ILE:HG23	1.62	0.62
1:A:79:CYS:HB3	1:A:87:PHE:CE1	2.33	0.62
1:A:265:ARG:HH11	1:A:277:MET:HG3	1.52	0.62
1:B:282:MET:O	1:B:284:CYS:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:O	1:A:227:MET:HE2	2.00	0.62
1:B:288:ASN:HD21	1:B:290:THR:CB	2.11	0.62
1:B:262:ILE:HG23	1:B:281:LEU:HD21	1.81	0.62
1:A:224:ASN:CA	1:A:227:MET:HE2	2.30	0.62
1:A:284:CYS:SG	1:A:285:VAL:HG23	2.38	0.62
1:A:284:CYS:CB	1:A:291:PRO:HB3	2.30	0.62
1:B:275:GLU:HG2	1:B:278:VAL:HG22	1.80	0.62
1:A:65:THR:CG2	1:A:92:LEU:H	2.09	0.62
1:B:288:ASN:HD21	1:B:290:THR:HB	1.65	0.62
1:B:340:VAL:HG23	1:B:341:LEU:CD2	2.30	0.62
1:A:437:LYS:HE3	1:A:446:SER:HB2	1.80	0.62
1:B:216:SER:OG	1:B:217:THR:N	2.33	0.62
1:A:152:TYR:CD2	1:A:279:TRP:HZ2	2.18	0.62
1:B:265:ARG:NH1	1:B:275:GLU:OE2	2.33	0.62
1:A:132:ARG:O	1:A:133:HIS:HB2	1.99	0.62
1:A:115:ASP:HB3	1:A:384:MET:HE2	1.81	0.62
1:A:400:LEU:HD23	1:A:400:LEU:C	2.19	0.62
1:B:86:ILE:HB	1:B:99:TYR:CD1	2.35	0.61
1:A:272:LYS:HE3	4:A:2039:HOH:O	2.00	0.61
1:B:340:VAL:O	1:B:341:LEU:HD23	2.00	0.61
1:B:449:THR:O	1:B:449:THR:HG22	2.00	0.61
1:A:381:LYS:O	1:A:382:ASN:OD1	2.18	0.61
1:A:59:PHE:CG	1:A:60:PRO:CD	2.81	0.61
1:B:493:ASP:HB3	4:B:2072:HOH:O	2.00	0.61
1:A:110:ASN:OD1	1:A:447:LYS:CB	2.45	0.61
1:A:59:PHE:CE2	1:A:62:ILE:CG2	2.84	0.61
1:A:95:LYS:HD2	1:A:397:HIS:CD2	2.35	0.61
2:A:580:HEM:HBD2	2:A:580:HEM:HHA	1.83	0.61
1:B:285:VAL:HG12	1:B:286:TYR:O	2.01	0.61
1:B:209:GLU:OE2	1:B:265:ARG:CZ	2.50	0.60
1:A:284:CYS:HB2	1:A:291:PRO:CB	2.30	0.60
1:A:361:LYS:HZ1	1:A:428:ILE:CG2	2.12	0.60
1:A:51:THR:HG23	1:A:52:PRO:HD2	1.83	0.60
1:A:55:VAL:O	1:A:57:HIS:HD2	1.83	0.60
1:B:57:HIS:ND1	1:B:59:PHE:O	2.34	0.60
1:B:380:VAL:CG2	1:B:397:HIS:O	2.50	0.60
1:A:82:LYS:CB	1:A:83:TYR:CD1	2.85	0.60
1:B:61:PHE:CE1	1:B:92:LEU:O	2.54	0.60
1:B:258:TYR:O	1:B:262:ILE:HG13	2.02	0.60
1:A:79:CYS:CB	1:A:87:PHE:CE2	2.85	0.60
1:A:277:MET:O	1:A:281:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:HG22	1:B:52:PRO:HD3	1.84	0.60
1:B:233:ASN:OD1	1:B:243:HIS:NE2	2.31	0.60
1:A:357:ASP:O	1:A:361:LYS:HG3	2.03	0.59
1:B:233:ASN:O	1:B:237:PRO:HD3	2.01	0.59
1:B:236:LEU:HD23	1:B:238:TRP:CZ2	2.37	0.59
1:A:59:PHE:CD2	1:A:60:PRO:HD2	2.38	0.59
1:A:51:THR:CG2	1:A:52:PRO:CD	2.80	0.59
1:A:389:THR:HG22	1:A:390:SER:H	1.65	0.59
1:B:394:PRO:O	1:B:397:HIS:HB2	2.02	0.59
1:A:51:THR:HG1	1:A:52:PRO:HD3	1.63	0.59
1:A:82:LYS:CB	1:A:83:TYR:CE1	2.85	0.59
1:B:212:SER:O	1:B:215:ASP:HB2	2.02	0.59
1:B:400:LEU:HD23	1:B:400:LEU:C	2.23	0.59
1:A:123:SER:N	1:A:124:PRO:HD2	2.18	0.58
1:A:435:ASP:CB	1:A:448:GLY:CA	2.80	0.58
1:A:246:LYS:NZ	4:A:2042:HOH:O	2.36	0.58
1:A:344:ASP:OD1	1:A:344:ASP:N	2.35	0.58
1:B:381:LYS:C	1:B:382:ASN:OD1	2.41	0.58
1:A:79:CYS:CB	1:A:87:PHE:CZ	2.85	0.58
1:B:87:PHE:CE1	1:B:98:VAL:HB	2.39	0.58
1:B:95:LYS:CD	1:B:397:HIS:CD2	2.84	0.58
1:B:402:SER:OG	1:B:405:VAL:HG23	2.04	0.58
1:B:340:VAL:C	1:B:341:LEU:HD23	2.23	0.58
3:B:590:VOR:C17	3:B:590:VOR:H21	2.32	0.58
1:A:51:THR:OG1	1:A:52:PRO:HD2	2.02	0.58
1:A:378:ARG:HH21	1:A:461:HIS:HD2	1.52	0.58
1:A:60:PRO:O	1:A:61:PHE:HB3	2.03	0.58
1:A:92:LEU:HD12	1:A:235:MET:CE	2.31	0.58
1:A:152:TYR:CB	1:A:279:TRP:HZ2	2.14	0.58
4:A:2085:HOH:O	1:B:510:ARG:NE	2.37	0.58
1:A:83:TYR:CD1	1:A:83:TYR:N	2.71	0.58
1:B:153:GLY:HA2	1:B:279:TRP:CD1	2.39	0.58
1:A:364:LYS:HE3	1:A:429:ALA:H	1.68	0.57
1:A:357:ASP:OD1	1:A:428:ILE:HG21	2.04	0.57
1:B:80:ARG:O	1:B:84:GLY:N	2.37	0.57
1:A:80:ARG:N	1:A:87:PHE:CZ	2.72	0.57
1:A:378:ARG:NH2	1:A:461:HIS:CD2	2.73	0.57
1:A:51:THR:CG2	1:A:52:PRO:HD2	2.34	0.57
1:A:86:ILE:HD13	1:A:99:TYR:HA	1.87	0.57
1:B:429:ALA:C	1:B:431:SER:H	2.08	0.57
1:B:456:PHE:HB3	1:B:463:CYS:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:CA	1:B:292:VAL:H	2.17	0.57
1:B:89:PHE:CE2	1:B:91:LEU:HG	2.40	0.57
1:B:209:GLU:CB	1:B:261:ILE:HD13	2.35	0.57
1:A:59:PHE:CD2	1:A:62:ILE:CG2	2.88	0.56
1:A:97:THR:N	1:A:398:ASN:O	2.26	0.56
1:B:387:ASP:OD1	1:B:387:ASP:N	2.39	0.56
1:B:433:GLU:OE1	1:B:448:GLY:HA3	2.05	0.56
1:B:453:TYR:CE1	1:B:455:PRO:HG3	2.41	0.56
1:A:106:ASP:OD1	1:A:110:ASN:ND2	2.36	0.56
1:A:477:THR:O	1:A:481:VAL:HG23	2.05	0.56
1:B:444:LEU:C	1:B:445:VAL:HG13	2.25	0.56
1:A:133:HIS:H	1:A:137:ASP:HB3	1.69	0.56
1:B:112:LYS:HD3	1:B:114:ARG:NE	2.20	0.56
1:B:98:VAL:HG11	1:B:100:LEU:HD21	1.86	0.56
1:B:277:MET:O	1:B:281:LEU:HG	2.05	0.56
1:A:282:MET:C	1:A:284:CYS:N	2.58	0.56
2:A:580:HEM:HBC2	2:A:580:HEM:CMC	2.35	0.56
1:A:224:ASN:HA	1:A:227:MET:CE	2.33	0.56
1:B:435:ASP:HB2	1:B:448:GLY:CA	2.36	0.56
1:A:357:ASP:CG	1:A:361:LYS:HE2	2.26	0.55
1:A:361:LYS:HZ1	1:A:428:ILE:HG22	1.64	0.55
1:A:99:TYR:CG	1:A:104:GLY:HA2	2.41	0.55
1:B:127:THR:HB	1:B:128:PRO:HD3	1.88	0.55
1:A:90:ILE:HG22	1:A:95:LYS:N	2.21	0.55
1:A:440:TYR:HE1	1:A:445:VAL:CG2	2.18	0.55
1:A:117:CYS:SG	1:A:119:GLU:CD	2.85	0.55
1:A:284:CYS:SG	1:A:291:PRO:HB3	2.46	0.55
1:B:89:PHE:HE2	1:B:91:LEU:HG	1.72	0.55
1:A:265:ARG:NH2	1:A:275:GLU:OE2	2.37	0.55
3:B:590:VOR:C21	3:B:590:VOR:C13	2.83	0.55
1:B:372:PRO:HD3	4:B:2045:HOH:O	2.05	0.55
1:A:231:PRO:O	1:A:234:PHE:HB2	2.07	0.54
1:B:153:GLY:N	1:B:279:TRP:HE1	2.04	0.54
1:A:440:TYR:CE1	1:A:445:VAL:CG2	2.90	0.54
1:B:123:SER:N	1:B:124:PRO:HD2	2.22	0.54
1:A:265:ARG:HH12	1:A:277:MET:CG	2.07	0.54
1:B:60:PRO:O	1:B:61:PHE:HB3	2.08	0.54
1:B:208:LYS:NZ	1:B:272:LYS:HD3	2.23	0.54
1:B:319:ILE:O	1:B:323:LEU:HG	2.08	0.54
1:A:53:PRO:CD	1:A:391:TYR:CE1	2.82	0.54
1:A:447:LYS:O	1:A:448:GLY:C	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:HB2	1:B:288:ASN:OD1	2.07	0.54
1:B:426:GLU:O	1:B:427:ASN:OD1	2.26	0.53
1:B:98:VAL:HG12	1:B:100:LEU:HD21	1.87	0.53
1:B:178:PRO:HA	1:B:181:GLN:HG2	1.90	0.53
1:B:297:ILE:O	1:B:301:MET:HG2	2.09	0.53
3:A:590:VOR:C21	3:A:590:VOR:C13	2.85	0.53
1:B:124:PRO:O	1:B:128:PRO:CD	2.56	0.53
3:A:590:VOR:H21	3:A:590:VOR:H17	1.89	0.53
1:A:90:ILE:HG23	1:A:95:LYS:HA	1.89	0.53
1:A:92:LEU:CD1	1:A:235:MET:CE	2.87	0.53
1:A:166:ILE:O	1:A:170:VAL:HG23	2.09	0.53
1:A:435:ASP:CG	1:A:448:GLY:HA3	2.29	0.53
1:B:160:ARG:HA	1:B:350:TYR:HB2	1.90	0.53
1:B:221:LEU:HD21	1:B:253:LYS:HD3	1.91	0.53
1:B:80:ARG:HA	1:B:84:GLY:O	2.09	0.53
1:B:433:GLU:CD	1:B:446:SER:OG	2.46	0.53
1:A:277:MET:CE	1:A:277:MET:CA	2.84	0.52
1:A:149:PHE:O	1:A:279:TRP:NE1	2.35	0.52
1:A:271:LYS:CG	1:A:272:LYS:N	2.72	0.52
1:A:433:GLU:HG2	1:A:434:ASP:N	2.18	0.52
1:A:450:ASN:N	1:A:450:ASN:HD22	2.07	0.52
1:B:172:SER:HB3	4:B:2004:HOH:O	2.09	0.52
1:B:338:ILE:O	1:B:341:LEU:O	2.28	0.52
1:A:311:SER:HB2	2:A:580:HEM:CAB	2.40	0.52
1:B:395:THR:HG22	1:B:395:THR:O	2.10	0.52
1:A:266:ARG:O	1:A:269:GLY:N	2.43	0.52
1:A:435:ASP:O	1:A:437:LYS:NZ	2.40	0.52
1:B:135:VAL:HG12	1:B:136:TYR:CG	2.45	0.52
1:B:95:LYS:HB2	1:B:397:HIS:CD2	2.45	0.51
1:A:52:PRO:HA	1:A:391:TYR:CD1	2.44	0.51
1:A:80:ARG:HA	1:A:87:PHE:CZ	2.45	0.51
1:A:62:ILE:HG13	1:A:63:GLY:N	2.24	0.51
1:A:378:ARG:HB2	1:A:399:VAL:CG2	2.39	0.51
1:B:109:LEU:HD13	1:B:458:ALA:HB3	1.92	0.51
1:B:110:ASN:OD1	1:B:447:LYS:HG3	2.10	0.51
1:B:162:TYR:CD1	1:B:204:SER:HB2	2.45	0.51
1:A:226:ASP:OD1	1:A:310:HIS:NE2	2.41	0.51
1:A:434:ASP:OD1	1:A:434:ASP:C	2.48	0.51
1:B:282:MET:C	1:B:284:CYS:N	2.63	0.51
1:A:59:PHE:CD2	1:A:60:PRO:O	2.64	0.51
1:B:357:ASP:OD2	1:B:361:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:HB3	1:B:291:PRO:HB3	1.93	0.51
1:A:90:ILE:H	1:A:90:ILE:CD1	1.98	0.50
1:B:135:VAL:HG12	1:B:136:TYR:CD2	2.47	0.50
1:B:463:CYS:HA	2:B:580:HEM:CHA	2.40	0.50
3:B:590:VOR:H21	3:B:590:VOR:H17	1.92	0.50
1:A:152:TYR:HB3	1:A:279:TRP:CE2	2.45	0.50
1:A:152:TYR:HD2	1:A:279:TRP:HZ2	1.57	0.50
1:A:435:ASP:OD2	1:A:448:GLY:HA3	2.11	0.50
1:B:403:PRO:HB3	1:B:454:LEU:HB2	1.94	0.50
1:A:494:GLY:HA2	4:A:2025:HOH:O	2.11	0.50
1:B:51:THR:CG2	1:B:52:PRO:HD3	2.40	0.50
1:A:169:GLU:OE1	4:A:2026:HOH:O	2.20	0.50
1:A:449:THR:C	1:A:450:ASN:HD22	2.15	0.50
1:B:112:LYS:CD	1:B:114:ARG:NE	2.74	0.50
1:B:166:ILE:O	1:B:170:VAL:HG23	2.11	0.50
1:B:277:MET:SD	1:B:277:MET:C	2.89	0.50
1:A:79:CYS:C	1:A:87:PHE:CE1	2.85	0.50
1:A:277:MET:C	1:A:279:TRP:H	2.15	0.50
1:B:275:GLU:O	1:B:277:MET:N	2.45	0.50
1:A:63:GLY:HA3	1:A:90:ILE:HD13	1.93	0.50
1:A:378:ARG:NH2	1:A:461:HIS:HD2	2.09	0.50
1:A:376:ILE:CG2	1:A:378:ARG:HH12	2.25	0.49
1:B:361:LYS:NZ	1:B:425:ASP:OD1	2.40	0.49
1:B:132:ARG:N	1:B:299:HIS:CE1	2.80	0.49
1:B:152:TYR:O	1:B:279:TRP:CE2	2.64	0.49
1:A:435:ASP:HB2	1:A:448:GLY:CA	2.40	0.49
1:A:90:ILE:N	1:A:90:ILE:CD1	2.67	0.49
1:A:108:ILE:HD12	1:A:401:SER:HB3	1.95	0.49
1:A:293:PRO:HG2	1:A:296:GLU:HG3	1.95	0.49
1:A:298:ALA:O	1:A:302:ILE:HG13	2.12	0.49
1:A:286:TYR:CE1	1:A:292:VAL:HG22	2.46	0.49
1:B:284:CYS:HA	1:B:292:VAL:HB	1.95	0.49
1:A:65:THR:HG21	1:A:92:LEU:N	2.14	0.49
1:A:446:SER:C	1:A:448:GLY:H	2.12	0.49
1:B:277:MET:O	1:B:277:MET:SD	2.70	0.49
1:B:292:VAL:HG12	1:B:297:ILE:CG1	2.43	0.49
1:A:55:VAL:CB	1:A:88:THR:O	2.61	0.49
1:A:400:LEU:C	1:A:400:LEU:CD2	2.80	0.49
1:B:439:ASP:OD1	1:B:441:GLY:N	2.40	0.49
1:A:471:LEU:O	1:A:475:THR:OG1	2.22	0.49
1:A:120:GLU:OE2	1:A:381:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:O	1:B:278:VAL:HG22	2.12	0.48
1:A:80:ARG:CA	1:A:87:PHE:HZ	2.26	0.48
1:B:276:ASP:O	1:B:279:TRP:HB3	2.13	0.48
1:A:97:THR:O	1:A:399:VAL:HA	2.14	0.48
1:B:262:ILE:HG23	1:B:281:LEU:CD2	2.43	0.48
1:B:336:GLU:OE1	1:B:358:LEU:HB3	2.13	0.48
1:B:350:TYR:CE2	1:B:354:GLN:NE2	2.82	0.48
1:B:493:ASP:CG	1:B:494:GLY:H	2.08	0.48
1:A:116:VAL:HB	1:A:378:ARG:HB3	1.95	0.48
1:B:377:ILE:O	1:B:378:ARG:NH1	2.43	0.48
1:B:284:CYS:SG	1:B:291:PRO:HB3	2.54	0.48
1:B:311:SER:HB2	2:B:580:HEM:CAB	2.43	0.48
1:B:202:SER:HA	1:B:206:GLN:HB2	1.96	0.48
1:B:364:LYS:HG2	1:B:424:TRP:CZ2	2.49	0.48
1:B:395:THR:O	1:B:395:THR:CG2	2.61	0.48
1:B:519:HIS:O	1:B:519:HIS:CG	2.65	0.48
1:A:144:MET:HE2	1:A:144:MET:HA	1.96	0.48
1:A:275:GLU:HG3	1:A:277:MET:CB	2.26	0.48
1:A:58:TRP:O	1:A:58:TRP:CD2	2.67	0.47
1:A:230:ALA:O	1:A:233:ASN:HB2	2.14	0.47
1:A:80:ARG:CA	1:A:87:PHE:CZ	2.97	0.47
1:B:169:GLU:OE2	1:B:203:ARG:NH1	2.45	0.47
1:B:224:ASN:O	1:B:227:MET:CE	2.62	0.47
1:B:482:ARG:O	1:B:518:ARG:HD2	2.13	0.47
1:B:281:LEU:HD23	1:B:297:ILE:HD13	1.95	0.47
1:B:379:ALA:HA	1:B:398:ASN:OD1	2.14	0.47
1:A:50:LYS:C	1:A:51:THR:HG22	2.31	0.47
1:A:273:ASP:HB3	1:A:274:SER:HB2	1.96	0.47
1:A:79:CYS:C	1:A:87:PHE:CZ	2.88	0.47
1:A:361:LYS:HZ3	1:A:428:ILE:CG2	2.16	0.47
1:B:275:GLU:C	1:B:277:MET:N	2.68	0.47
1:B:112:LYS:O	1:B:116:VAL:HG22	2.14	0.47
1:A:79:CYS:HB3	1:A:87:PHE:CD2	2.49	0.47
1:A:294:ASP:OD1	4:A:2050:HOH:O	2.21	0.47
1:A:372:PRO:HG2	1:A:373:ILE:HD12	1.97	0.47
1:A:437:LYS:CE	1:A:446:SER:HB2	2.44	0.47
1:B:86:ILE:HA	1:B:98:VAL:O	2.15	0.47
1:B:136:TYR:OH	2:B:580:HEM:CBD	2.62	0.47
1:B:224:ASN:CA	1:B:227:MET:CE	2.77	0.47
1:B:262:ILE:CG1	1:B:277:MET:CE	2.66	0.47
1:B:373:ILE:N	1:B:373:ILE:CD1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:OH	1:B:375:SER:OG	2.28	0.47
1:A:293:PRO:HD2	1:A:296:GLU:OE1	2.15	0.47
1:A:356:LEU:HB3	1:A:359:HIS:HB2	1.97	0.47
1:B:71:ASP:OD1	1:B:73:TYR:N	2.45	0.47
1:B:98:VAL:CG1	1:B:100:LEU:CD2	2.87	0.47
1:B:153:GLY:N	1:B:279:TRP:CD1	2.83	0.47
1:A:120:GLU:OE1	1:A:381:LYS:HE2	2.14	0.46
1:A:385:ALA:N	4:A:2071:HOH:O	2.39	0.46
1:A:152:TYR:HD2	1:A:279:TRP:CZ2	2.32	0.46
1:B:153:GLY:HA2	1:B:279:TRP:CG	2.50	0.46
1:A:59:PHE:HB3	1:A:62:ILE:HG12	1.97	0.46
1:A:83:TYR:N	1:A:83:TYR:HD1	2.13	0.46
1:A:160:ARG:HG2	1:A:350:TYR:CG	2.50	0.46
1:A:265:ARG:NH1	1:A:278:VAL:HG22	2.30	0.46
1:B:132:ARG:N	1:B:299:HIS:ND1	2.63	0.46
1:A:77:PHE:HE1	1:A:405:VAL:HG13	1.81	0.46
1:A:86:ILE:HD11	1:A:99:TYR:CE1	2.45	0.46
1:B:453:TYR:CZ	1:B:455:PRO:HG2	2.50	0.46
1:A:381:LYS:HB3	4:A:2006:HOH:O	2.16	0.46
1:A:79:CYS:HB2	1:A:87:PHE:CE2	2.50	0.46
1:B:149:PHE:CD1	1:B:283:SER:OG	2.68	0.46
1:B:275:GLU:O	1:B:276:ASP:C	2.54	0.46
1:A:288:ASN:ND2	4:A:2051:HOH:O	2.49	0.46
1:B:140:ASN:O	1:B:144:MET:HG2	2.15	0.46
1:B:145:GLU:OE1	1:B:286:TYR:HA	2.15	0.46
1:B:281:LEU:HD23	1:B:297:ILE:CD1	2.45	0.46
1:A:59:PHE:CE2	1:A:60:PRO:O	2.69	0.46
1:A:156:SER:O	1:A:160:ARG:HG3	2.15	0.46
1:B:453:TYR:CZ	1:B:455:PRO:CG	2.99	0.46
1:A:277:MET:SD	1:A:281:LEU:HD21	2.56	0.46
1:B:122:TYR:OH	3:B:590:VOR:H24	2.16	0.46
1:B:262:ILE:HA	1:B:277:MET:CE	2.47	0.46
1:B:374:HIS:CE1	1:B:375:SER:HG	2.31	0.46
1:B:119:GLU:O	1:B:123:SER:HB2	2.16	0.45
1:A:114:ARG:HG3	1:A:115:ASP:N	2.31	0.45
1:A:108:ILE:HD13	1:A:399:VAL:HB	1.98	0.45
1:A:133:HIS:H	1:A:137:ASP:CB	2.30	0.45
1:A:152:TYR:CD2	1:A:279:TRP:CZ2	3.01	0.45
1:A:424:TRP:C	1:A:426:GLU:N	2.69	0.45
1:B:131:GLY:HA3	1:B:299:HIS:ND1	2.32	0.45
1:A:59:PHE:CD1	1:A:60:PRO:CD	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:HB2	2:B:580:HEM:HAB	1.99	0.45
1:A:376:ILE:HG22	1:A:378:ARG:NH1	2.31	0.45
1:A:436:GLU:C	1:A:437:LYS:HD2	2.37	0.45
1:B:241:LEU:HB3	1:B:242:PRO:HD2	1.99	0.45
1:B:472:GLN:O	1:B:476:ILE:HG13	2.17	0.45
1:A:286:TYR:CD1	1:A:290:THR:HG23	2.52	0.44
1:A:55:VAL:HG21	1:A:89:PHE:HB2	1.93	0.44
2:A:580:HEM:HBC2	2:A:580:HEM:HMC2	1.98	0.44
1:B:338:ILE:HD13	1:B:345:LEU:HD21	1.98	0.44
1:A:277:MET:C	1:A:279:TRP:N	2.71	0.44
1:B:217:THR:HG21	4:B:2038:HOH:O	2.17	0.44
1:A:90:ILE:CD1	1:A:90:ILE:O	2.65	0.44
1:A:378:ARG:HH21	1:A:461:HIS:CD2	2.30	0.44
1:B:208:LYS:N	4:B:2034:HOH:O	2.44	0.44
1:A:225:LEU:HD22	1:A:254:LEU:CD1	2.48	0.44
1:A:384:MET:HG3	1:A:393:ILE:HB	2.00	0.44
1:A:61:PHE:HZ	1:A:235:MET:HE3	1.83	0.44
1:A:80:ARG:HA	1:A:87:PHE:CE1	2.53	0.44
1:A:297:ILE:O	1:A:301:MET:HG2	2.17	0.44
1:B:108:ILE:HD12	1:B:401:SER:HB2	1.99	0.44
1:B:135:VAL:HA	1:B:143:LEU:CD1	2.48	0.44
1:B:374:HIS:CE1	1:B:375:SER:OG	2.70	0.44
1:A:428:ILE:HD12	1:A:429:ALA:N	2.32	0.44
1:B:519:HIS:C	1:B:519:HIS:CD2	2.90	0.44
1:B:210:VAL:HG13	1:B:218:PHE:CD2	2.52	0.44
1:B:424:TRP:HE3	1:B:427:ASN:O	2.01	0.44
1:B:124:PRO:O	1:B:128:PRO:HD2	2.17	0.44
1:A:79:CYS:HB3	1:A:87:PHE:CD1	2.53	0.43
1:A:213:LYS:HB3	1:A:218:PHE:CD1	2.53	0.43
1:B:515:PHE:CD1	1:B:515:PHE:C	2.91	0.43
1:A:84:GLY:O	1:A:87:PHE:CE1	2.71	0.43
1:A:340:VAL:HG11	1:A:355:LYS:CB	2.48	0.43
1:B:106:ASP:HA	1:B:449:THR:HG21	1.95	0.43
1:A:123:SER:O	1:A:127:THR:OG1	2.31	0.43
1:A:124:PRO:O	1:A:128:PRO:CG	2.66	0.43
1:A:163:VAL:HB	1:A:164:PRO:CD	2.47	0.43
1:A:424:TRP:C	1:A:426:GLU:H	2.21	0.43
1:A:72:PRO:O	1:A:75:PHE:HB3	2.18	0.43
1:A:284:CYS:SG	1:A:285:VAL:CG2	3.07	0.43
1:B:51:THR:CB	1:B:52:PRO:HD3	2.44	0.43
1:B:153:GLY:CA	1:B:279:TRP:NE1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:C	1:B:400:LEU:CD2	2.87	0.43
1:B:493:ASP:N	4:B:2072:HOH:O	2.42	0.43
1:A:61:PHE:HZ	1:A:235:MET:CE	2.32	0.43
1:B:98:VAL:HG12	1:B:100:LEU:HD23	2.00	0.43
1:A:233:ASN:OD1	1:A:237:PRO:HA	2.19	0.43
1:A:386:VAL:HG23	1:A:389:THR:H	1.84	0.43
1:B:135:VAL:HG12	1:B:136:TYR:N	2.33	0.43
1:B:292:VAL:CG1	1:B:297:ILE:HG12	2.49	0.43
1:B:435:ASP:CB	1:B:448:GLY:HA3	2.46	0.43
1:A:90:ILE:HA	1:A:94:LYS:O	2.19	0.43
1:A:285:VAL:HA	1:A:290:THR:O	2.19	0.43
1:A:418:GLU:OE1	1:A:418:GLU:HA	2.19	0.43
1:B:363:ILE:HD11	1:B:474:GLY:HA2	2.01	0.43
1:A:140:ASN:HD21	1:A:460:ARG:HH11	1.66	0.42
1:A:318:TRP:CE2	1:A:507:PRO:HG3	2.54	0.42
1:A:357:ASP:OD2	1:A:361:LYS:CE	2.62	0.42
1:B:92:LEU:HD23	1:B:92:LEU:N	2.33	0.42
1:B:215:ASP:OD1	4:B:2031:HOH:O	2.21	0.42
1:B:344:ASP:OD1	1:B:344:ASP:N	2.51	0.42
1:B:477:THR:O	1:B:481:VAL:HG23	2.18	0.42
1:B:491:GLY:C	1:B:492:VAL:HG23	2.39	0.42
1:B:502:SER:HB3	4:B:2074:HOH:O	2.20	0.42
1:B:167:THR:O	1:B:171:GLU:HG3	2.19	0.42
1:B:236:LEU:CD2	1:B:238:TRP:CH2	3.03	0.42
1:A:127:THR:N	1:A:128:PRO:CD	2.82	0.42
1:A:364:LYS:HE3	1:A:429:ALA:N	2.33	0.42
1:B:132:ARG:H	1:B:299:HIS:HE1	1.65	0.42
1:B:152:TYR:CA	1:B:279:TRP:CZ2	3.03	0.42
2:B:580:HEM:HBB2	2:B:580:HEM:CMB	2.50	0.42
1:A:275:GLU:OE2	1:A:277:MET:HB3	2.20	0.42
1:A:380:VAL:HG23	1:A:397:HIS:O	2.19	0.42
1:A:80:ARG:N	1:A:87:PHE:HZ	2.16	0.42
1:A:90:ILE:CG2	1:A:95:LYS:CA	2.81	0.42
1:A:120:GLU:OE2	1:A:381:LYS:CE	2.67	0.42
1:B:393:ILE:HA	1:B:394:PRO:HD2	1.93	0.42
1:A:277:MET:C	1:A:277:MET:SD	2.98	0.42
1:A:307:ALA:O	1:A:311:SER:OG	2.28	0.42
1:B:339:ARG:NH2	4:B:2052:HOH:O	2.53	0.42
1:B:489:LEU:HG	1:B:490:PRO:HD2	2.02	0.42
1:A:115:ASP:HB3	1:A:384:MET:HE3	1.98	0.42
1:A:344:ASP:O	1:A:345:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:N	1:B:164:PRO:CD	2.82	0.42
1:B:224:ASN:O	1:B:227:MET:HE3	2.19	0.42
1:B:288:ASN:ND2	1:B:290:THR:CB	2.77	0.42
1:B:413:PHE:HB3	1:B:423:ARG:NH1	2.35	0.42
1:A:82:LYS:HB2	1:A:83:TYR:HD1	1.74	0.42
1:A:393:ILE:HA	1:A:394:PRO:HD3	1.82	0.42
1:B:122:TYR:OH	3:B:590:VOR:C24	2.68	0.42
1:B:364:LYS:HD3	1:B:424:TRP:CZ3	2.55	0.42
1:B:377:ILE:HG23	1:B:399:VAL:O	2.19	0.42
1:A:91:LEU:O	1:A:92:LEU:HB2	2.20	0.42
1:B:284:CYS:C	1:B:292:VAL:H	2.22	0.42
1:B:288:ASN:OD1	1:B:290:THR:N	2.43	0.42
1:B:373:ILE:HD12	1:B:373:ILE:H	1.83	0.42
1:A:187:PHE:O	1:A:512:PHE:HA	2.20	0.42
1:B:197:THR:HG21	1:B:313:SER:HA	2.01	0.42
1:B:446:SER:C	1:B:448:GLY:H	2.21	0.42
1:A:82:LYS:HB2	1:A:83:TYR:HE1	1.79	0.41
1:A:350:TYR:O	1:A:354:GLN:NE2	2.53	0.41
1:B:224:ASN:C	1:B:227:MET:HE2	2.41	0.41
1:A:59:PHE:CD2	1:A:60:PRO:CD	3.04	0.41
1:A:59:PHE:CZ	1:A:60:PRO:HD2	2.54	0.41
1:A:340:VAL:HG11	1:A:355:LYS:HB2	2.02	0.41
1:A:436:GLU:O	1:A:437:LYS:HD2	2.20	0.41
1:B:284:CYS:SG	1:B:291:PRO:CB	3.08	0.41
1:B:380:VAL:HG12	1:B:395:THR:HA	2.01	0.41
1:A:153:GLY:HA3	1:A:279:TRP:CD1	2.55	0.41
1:A:447:LYS:HA	1:A:459:GLY:N	2.28	0.41
1:B:123:SER:O	1:B:127:THR:OG1	2.26	0.41
1:A:100:LEU:O	1:A:104:GLY:HA3	2.21	0.41
1:A:286:TYR:HD1	1:A:290:THR:O	2.03	0.41
1:A:349:THR:HG21	4:A:2065:HOH:O	2.19	0.41
1:A:395:THR:C	1:A:397:HIS:H	2.23	0.41
2:A:580:HEM:CMB	2:A:580:HEM:HBB2	2.50	0.41
1:B:377:ILE:HG22	1:B:378:ARG:N	2.36	0.41
1:B:493:ASP:CB	4:B:2072:HOH:O	2.66	0.41
1:A:277:MET:HB2	1:A:277:MET:HE3	1.93	0.41
1:A:318:TRP:CD1	1:A:370:HIS:HB3	2.56	0.41
1:B:88:THR:HA	1:B:97:THR:HA	2.03	0.41
1:B:105:ASN:O	1:B:109:LEU:HG	2.21	0.41
1:B:130:PHE:CD1	1:B:303:ALA:HA	2.56	0.41
1:B:302:ILE:O	1:B:306:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ALA:HB1	1:B:431:SER:CB	2.50	0.41
1:B:488:ASN:HD22	1:B:493:ASP:HA	1.85	0.41
1:A:64:SER:O	1:A:67:SER:HB3	2.20	0.41
1:B:404:GLY:O	1:B:408:ARG:CG	2.65	0.41
1:A:55:VAL:HG22	1:A:89:PHE:CA	2.46	0.41
1:A:79:CYS:O	1:A:87:PHE:CE1	2.74	0.41
1:A:138:CYS:HB2	1:A:139:PRO:HD2	2.03	0.41
1:A:185:GLY:HA3	1:A:515:PHE:CE2	2.55	0.41
1:A:213:LYS:O	1:A:216:SER:N	2.53	0.41
1:A:285:VAL:HA	1:A:291:PRO:HA	2.02	0.41
1:A:290:THR:HG23	1:A:290:THR:O	2.21	0.41
1:A:376:ILE:CG2	1:A:378:ARG:NH1	2.84	0.41
1:A:434:ASP:OD1	1:A:434:ASP:O	2.39	0.41
1:A:469:ALA:O	1:A:473:LEU:HG	2.21	0.41
1:B:112:LYS:HD2	1:B:114:ARG:CZ	2.51	0.41
1:B:208:LYS:HZ2	1:B:272:LYS:HD3	1.86	0.41
1:B:364:LYS:HG3	1:B:453:TYR:OH	2.21	0.41
1:B:374:HIS:ND1	1:B:375:SER:OG	2.43	0.41
1:B:519:HIS:O	1:B:519:HIS:CD2	2.74	0.41
1:A:75:PHE:HZ	1:A:89:PHE:CG	2.39	0.41
1:B:110:ASN:ND2	1:B:449:THR:OG1	2.53	0.41
1:A:101:GLY:O	1:A:105:ASN:N	2.45	0.40
1:A:106:ASP:HB2	1:A:449:THR:HB	2.04	0.40
1:B:106:ASP:N	1:B:449:THR:HG21	2.36	0.40
1:B:292:VAL:HA	1:B:293:PRO:HD2	1.87	0.40
1:A:96:THR:HG22	1:A:398:ASN:HB2	2.04	0.40
1:A:114:ARG:CG	1:A:115:ASP:OD1	2.66	0.40
1:A:123:SER:N	1:A:124:PRO:CD	2.84	0.40
1:A:271:LYS:HG3	1:A:272:LYS:H	1.86	0.40
1:B:57:HIS:CE1	1:B:59:PHE:O	2.75	0.40
1:B:62:ILE:O	1:B:65:THR:HG22	2.21	0.40
1:B:128:PRO:O	1:B:251:GLN:HG3	2.20	0.40
1:B:429:ALA:HB1	1:B:431:SER:HB2	2.03	0.40
1:A:453:TYR:CZ	1:A:455:PRO:HG2	2.57	0.40
1:A:279:TRP:O	1:A:283:SER:HB3	2.21	0.40
1:A:499:ASP:HB2	1:A:508:LEU:HA	2.03	0.40
1:A:52:PRO:O	1:A:53:PRO:C	2.59	0.40
1:B:106:ASP:HB2	1:B:449:THR:CB	2.51	0.40
1:B:193:ILE:HD13	1:B:193:ILE:HA	1.88	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	468/470 (100%)	447 (96%)	18 (4%)	3 (1%)	25	34
1	B	468/470 (100%)	454 (97%)	12 (3%)	2 (0%)	34	46
All	All	936/940 (100%)	901 (96%)	30 (3%)	5 (0%)	29	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	433	GLU
1	B	51	THR
1	A	135	VAL
1	B	135	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/411 (100%)	384 (93%)	27 (7%)	16	22
1	B	411/411 (100%)	392 (95%)	19 (5%)	27	36
All	All	822/822 (100%)	776 (94%)	46 (6%)	21	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	62	ILE
1	A	83	TYR
1	A	90	ILE
1	A	91	LEU
1	A	92	LEU
1	A	99	TYR
1	A	152	TYR
1	A	218	PHE
1	A	238	TRP
1	A	252	ARG
1	A	270	SER
1	A	274	SER
1	A	278	VAL
1	A	282	MET
1	A	283	SER
1	A	389	THR
1	A	390	SER
1	A	399	VAL
1	A	410	GLU
1	A	428	ILE
1	A	434	ASP
1	A	444	LEU
1	A	450	ASN
1	A	462	ARG
1	A	510	ARG
1	A	519	HIS
1	B	51	THR
1	B	86	ILE
1	B	91	LEU
1	B	99	TYR
1	B	155	THR
1	B	218	PHE
1	B	263	LYS
1	B	265	ARG
1	B	270	SER
1	B	276	ASP
1	B	277	MET
1	B	284	CYS
1	B	341	LEU
1	B	387	ASP
1	B	389	THR
1	B	431	SER

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Mol	Chain	Res	Type
1	B	434	ASP
1	B	489	LEU
1	B	519	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	140	ASN
1	A	398	ASN
1	A	450	ASN
1	A	461	HIS
1	B	183	HIS
1	B	519	HIS

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	580	1,3	41,50,50	1.71	9 (21%)	45,82,82	1.88	9 (20%)
3	VOR	A	590	2	24,27,27	2.22	4 (16%)	33,39,39	2.47	10 (30%)
3	VOR	B	590	2	24,27,27	1.95	5 (20%)	33,39,39	2.55	12 (36%)
2	HEM	A	580	1,3	41,50,50	1.94	12 (29%)	45,82,82	2.06	11 (24%)

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	HEM	B	580	1,3	-	2/12/54/54	-
3	VOR	A	590	2	-	4/21/21/21	0/3/3/3
3	VOR	B	590	2	-	2/21/21/21	0/3/3/3
2	HEM	A	580	1,3	-	3/12/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	590	VOR	C13-C16	6.90	1.49	1.38
3	A	590	VOR	C18-C15	6.49	1.49	1.38
2	A	580	HEM	C1B-NB	-5.57	1.30	1.40
3	B	590	VOR	C18-C15	5.46	1.47	1.38
2	A	580	HEM	C4D-ND	-4.84	1.32	1.40
3	B	590	VOR	C13-C16	4.69	1.45	1.38
2	B	580	HEM	C1B-NB	-4.63	1.32	1.40
2	A	580	HEM	C4B-NB	-3.66	1.31	1.38
2	B	580	HEM	C4D-ND	-3.60	1.34	1.40
3	A	590	VOR	N7-N5	3.54	1.40	1.35
2	A	580	HEM	C1D-ND	-3.45	1.31	1.38
2	B	580	HEM	C4B-NB	-3.37	1.31	1.38
3	B	590	VOR	C21-N5	-3.19	1.30	1.33
2	A	580	HEM	FE-ND	-3.17	1.81	1.96
2	A	580	HEM	C3C-C2C	-3.01	1.36	1.40
2	A	580	HEM	C1B-C2B	-3.01	1.38	1.44
3	B	590	VOR	C10-C11	-2.98	1.51	1.56
2	B	580	HEM	C1D-ND	-2.95	1.32	1.38
2	B	580	HEM	C1B-C2B	-2.76	1.39	1.44
2	B	580	HEM	C3C-C2C	-2.75	1.36	1.40
2	A	580	HEM	C2C-C1C	-2.69	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	HEM	FE-ND	-2.63	1.83	1.96
2	A	580	HEM	C3D-C2D	-2.55	1.31	1.36
3	B	590	VOR	C10-C13	-2.40	1.49	1.53
2	B	580	HEM	O2A-CGA	-2.29	1.23	1.30
2	A	580	HEM	O2D-CGD	-2.26	1.23	1.30
2	A	580	HEM	C1A-CHA	-2.10	1.35	1.41
3	A	590	VOR	C10-C11	-2.06	1.52	1.56
2	B	580	HEM	C2C-C1C	-2.05	1.37	1.42
2	A	580	HEM	C4A-CHB	-2.05	1.35	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	590	VOR	C21-N8-C25	7.01	110.23	102.34
3	A	590	VOR	C21-N8-C25	6.47	109.63	102.34
2	A	580	HEM	CHC-C4B-NB	6.05	131.01	124.43
3	B	590	VOR	N8-C21-N5	-5.32	105.81	112.24
2	A	580	HEM	CHD-C1D-ND	5.16	130.03	124.43
2	B	580	HEM	CHC-C4B-NB	5.05	129.92	124.43
3	A	590	VOR	C23-N9-C24	5.04	122.26	115.80
3	A	590	VOR	N9-C24-N6	-4.98	122.22	127.70
3	B	590	VOR	C23-N9-C24	4.94	122.13	115.80
3	A	590	VOR	N8-C21-N5	-4.94	106.27	112.24
3	A	590	VOR	C19-C16-C13	-4.81	118.79	124.00
3	B	590	VOR	N9-C24-N6	-4.57	122.68	127.70
2	B	580	HEM	CHB-C1B-NB	4.17	129.54	124.38
3	B	590	VOR	C13-C10-C11	3.97	116.56	110.74
2	A	580	HEM	C1B-NB-C4B	3.96	109.16	105.07
2	B	580	HEM	CHD-C1D-ND	3.88	128.65	124.43
2	A	580	HEM	CHB-C1B-NB	3.86	129.14	124.38
2	B	580	HEM	CHA-C4D-ND	3.72	128.97	124.38
2	A	580	HEM	CHA-C4D-ND	3.66	128.90	124.38
2	A	580	HEM	CHD-C1D-C2D	-3.62	119.33	124.98
2	B	580	HEM	C1B-NB-C4B	3.54	108.72	105.07
2	B	580	HEM	CHA-C4D-C3D	-3.49	118.77	125.33
3	B	590	VOR	C12-C10-C13	-3.32	101.37	109.49
3	A	590	VOR	C16-C19-C22	3.26	120.04	116.62
3	B	590	VOR	C19-C16-C13	-3.10	120.64	124.00
3	B	590	VOR	C18-C23-N9	-3.09	118.25	121.72
3	B	590	VOR	C16-C19-C22	2.95	119.72	116.62
3	B	590	VOR	C17-C20-C22	2.82	121.28	118.36
3	A	590	VOR	C17-C20-C22	2.69	121.15	118.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	580	HEM	O2A-CGA-O1A	-2.66	116.66	123.30
2	A	580	HEM	CHA-C4D-C3D	-2.66	120.34	125.33
2	A	580	HEM	CAD-C3D-C4D	2.61	129.22	124.66
2	A	580	HEM	O2D-CGD-CBD	2.51	122.10	114.03
2	A	580	HEM	CHB-C1B-C2B	-2.49	119.83	126.72
3	B	590	VOR	O4-C10-C13	2.48	110.63	107.11
2	B	580	HEM	CHB-C1B-C2B	-2.37	120.16	126.72
3	B	590	VOR	C20-C22-C19	-2.34	120.25	123.29
2	A	580	HEM	O2D-CGD-O1D	-2.30	117.58	123.30
3	A	590	VOR	C10-C13-C16	-2.26	119.99	123.07
3	A	590	VOR	C17-C13-C16	2.23	118.87	116.10
2	B	580	HEM	C4D-C3D-C2D	-2.21	103.68	106.90
3	A	590	VOR	C18-C23-N9	-2.12	119.34	121.72

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	590	VOR	C10-C12-N5-C21
3	B	590	VOR	C10-C12-N5-C21
2	A	580	HEM	C4D-C3D-CAD-CBD
2	A	580	HEM	C2D-C3D-CAD-CBD
3	A	590	VOR	C10-C12-N5-N7
3	B	590	VOR	C10-C12-N5-N7
3	A	590	VOR	C10-C11-C15-C18
2	B	580	HEM	CAD-CBD-CGD-O1D
3	A	590	VOR	C10-C11-C15-N6
2	A	580	HEM	CAA-CBA-CGA-O1A
2	B	580	HEM	CAD-CBD-CGD-O2D

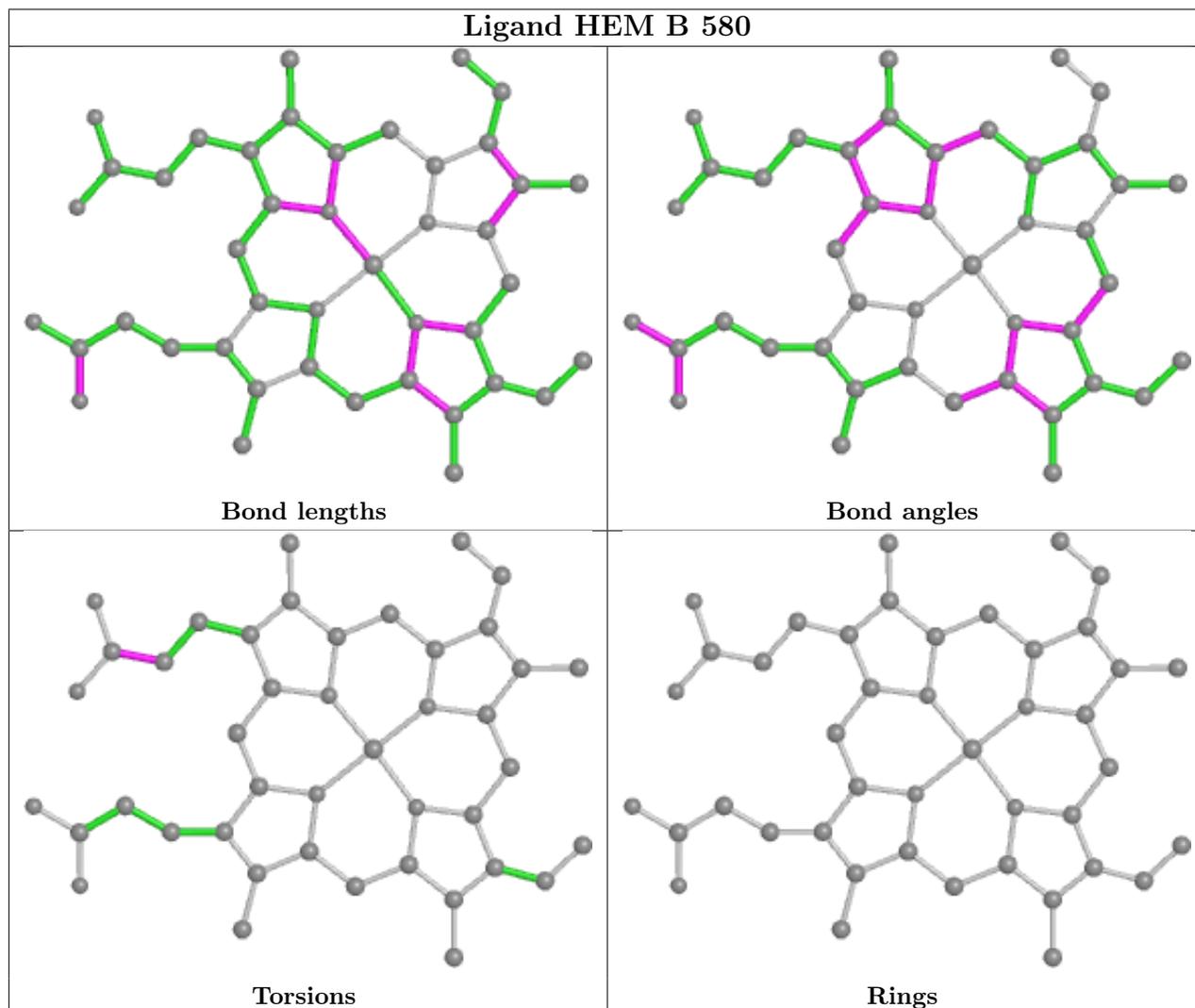
There are no ring outliers.

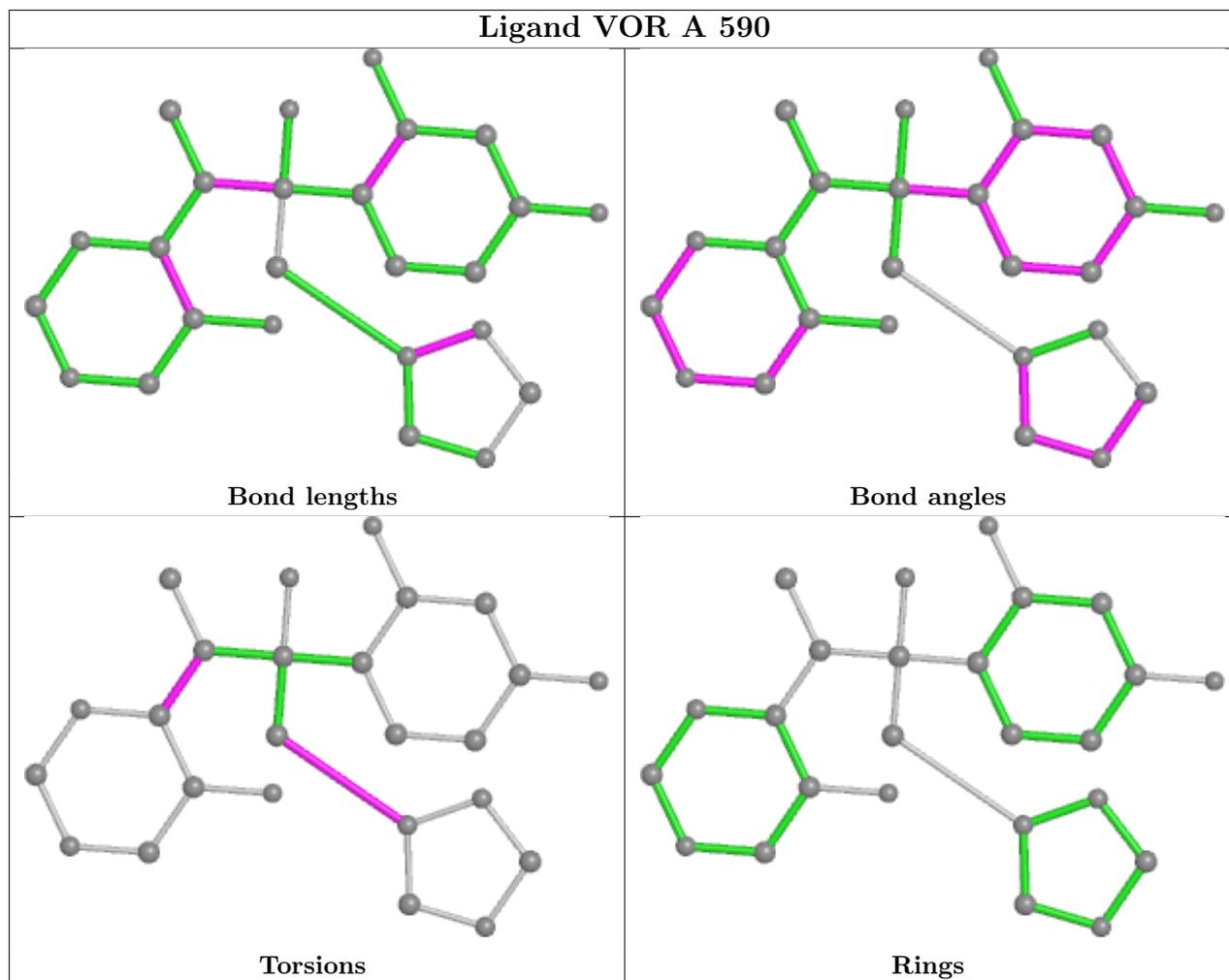
4 monomers are involved in 23 short contacts:

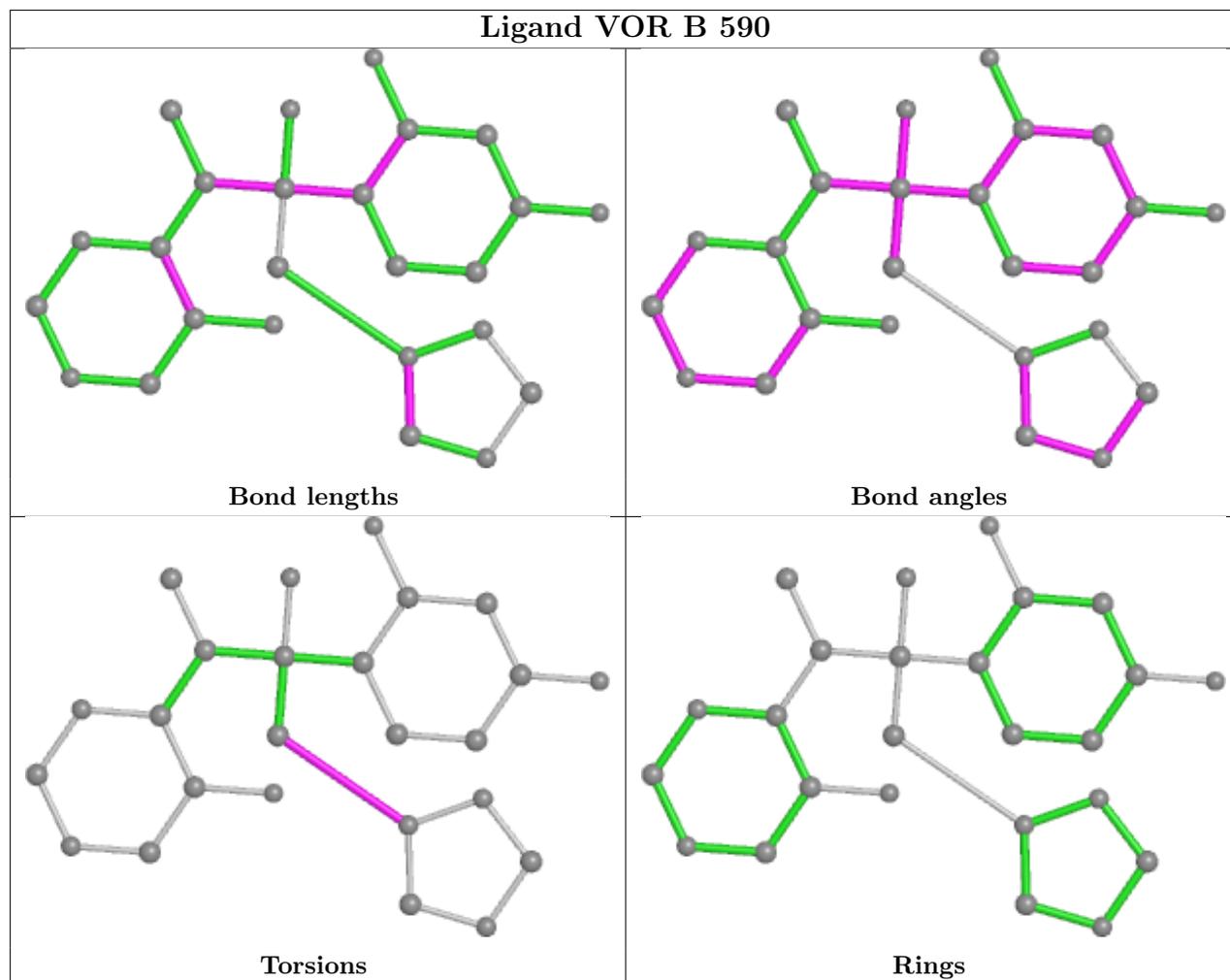
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	580	HEM	8	0
3	A	590	VOR	4	0
3	B	590	VOR	6	0
2	A	580	HEM	5	0

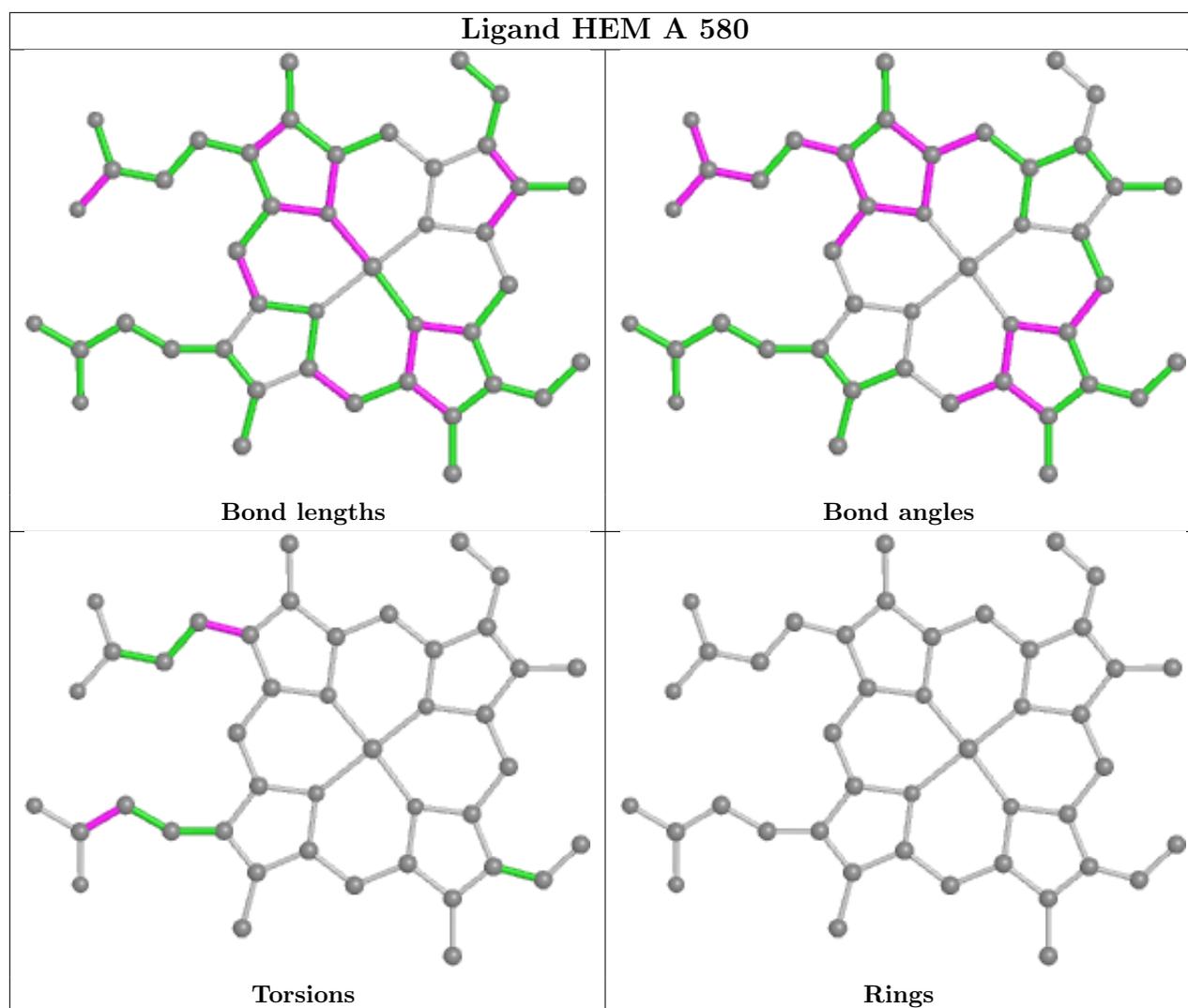
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/470 (100%)	0.78	65 (13%) 2 3	44, 70, 124, 189	0
1	B	470/470 (100%)	0.87	93 (19%) 1 1	47, 78, 123, 205	0
All	All	940/940 (100%)	0.83	158 (16%) 1 1	44, 74, 124, 205	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ILE	14.6
1	A	427	ASN	14.3
1	B	429	ALA	11.3
1	A	58	TRP	10.7
1	B	427	ASN	10.5
1	B	432	ALA	10.4
1	A	431	SER	9.7
1	A	432	ALA	7.4
1	A	428	ILE	7.0
1	B	241	LEU	7.0
1	A	59	PHE	6.5
1	A	429	ALA	6.5
1	B	430	ALA	6.4
1	A	56	PHE	6.2
1	B	60	PRO	6.0
1	A	60	PRO	5.8
1	A	284	CYS	5.6
1	B	50	LYS	5.4
1	B	431	SER	5.4
1	B	519	HIS	4.9
1	B	269	GLY	4.9
1	B	447	LYS	4.8
1	B	59	PHE	4.5
1	B	58	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	PHE	4.4
1	A	426	GLU	4.2
1	B	267	GLN	4.1
1	B	508	LEU	4.1
1	A	303	ALA	4.1
1	B	440	TYR	4.0
1	B	433	GLU	4.0
1	A	50	LYS	4.0
1	B	391	TYR	3.9
1	B	438	VAL	3.9
1	B	392	VAL	3.9
1	A	390	SER	3.8
1	B	283	SER	3.8
1	A	57	HIS	3.8
1	A	304	LEU	3.8
1	B	303	ALA	3.7
1	B	56	PHE	3.7
1	B	426	GLU	3.7
1	A	270	SER	3.7
1	A	388	GLY	3.5
1	A	279	TRP	3.5
1	B	284	CYS	3.4
1	A	62	ILE	3.3
1	A	307	ALA	3.3
1	A	392	VAL	3.3
1	B	305	LEU	3.3
1	B	319	ILE	3.3
1	A	391	TYR	3.2
1	A	319	ILE	3.2
1	A	152	TYR	3.2
1	B	387	ASP	3.1
1	B	268	ALA	3.1
1	B	437	LYS	3.1
1	B	311	SER	3.1
1	A	433	GLU	3.1
1	A	400	LEU	3.1
1	B	98	VAL	3.0
1	A	387	ASP	3.0
1	B	246	LYS	3.0
1	B	477	THR	3.0
1	B	410	GLU	3.0
1	B	304	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	3.0
1	A	98	VAL	3.0
1	A	376	ILE	3.0
1	B	400	LEU	3.0
1	B	401	SER	2.9
1	B	227	MET	2.9
1	B	306	MET	2.9
1	B	399	VAL	2.8
1	B	57	HIS	2.8
1	B	376	ILE	2.8
1	B	81	ALA	2.8
1	A	246	LYS	2.8
1	A	384	MET	2.8
1	B	99	TYR	2.8
1	B	312	SER	2.8
1	A	430	ALA	2.8
1	A	469	ALA	2.7
1	B	476	ILE	2.7
1	A	114	ARG	2.7
1	B	390	SER	2.7
1	A	268	ALA	2.7
1	A	302	ILE	2.7
1	B	113	LEU	2.7
1	A	205	LEU	2.7
1	B	313	SER	2.6
1	A	93	GLY	2.6
1	A	306	MET	2.6
1	B	279	TRP	2.6
1	B	375	SER	2.6
1	B	139	PRO	2.6
1	A	410	GLU	2.6
1	B	308	GLY	2.6
1	B	492	VAL	2.6
1	A	373	ILE	2.6
1	B	473	LEU	2.6
1	A	363	ILE	2.6
1	A	290	THR	2.6
1	B	366	THR	2.6
1	A	411	GLU	2.6
1	B	63	GLY	2.5
1	B	373	ILE	2.5
1	B	472	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	383	PRO	2.5
1	A	63	GLY	2.5
1	A	131	GLY	2.5
1	A	300	MET	2.5
1	A	477	THR	2.5
1	A	311	SER	2.4
1	B	411	GLU	2.4
1	A	445	VAL	2.4
1	A	113	LEU	2.4
1	B	82	LYS	2.3
1	B	238	TRP	2.3
1	B	371	ALA	2.3
1	A	61	PHE	2.3
1	B	315	THR	2.3
1	B	310	HIS	2.3
1	B	367	LEU	2.3
1	B	386	VAL	2.3
1	A	375	SER	2.3
1	B	54	VAL	2.2
1	A	377	ILE	2.2
1	B	51	THR	2.2
1	A	401	SER	2.2
1	A	476	ILE	2.2
1	B	302	ILE	2.2
1	B	277	MET	2.2
1	A	201	ALA	2.2
1	B	316	ALA	2.2
1	B	202	SER	2.2
1	B	197	THR	2.2
1	B	206	GLN	2.1
1	B	362	VAL	2.1
1	B	314	SER	2.1
1	A	305	LEU	2.1
1	A	227	MET	2.1
1	A	316	ALA	2.1
1	A	241	LEU	2.1
1	B	140	ASN	2.1
1	B	388	GLY	2.1
1	A	463	CYS	2.1
1	B	97	THR	2.1
1	B	266	ARG	2.1
1	A	232	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	ALA	2.1
1	B	363	ILE	2.0
1	B	253	LYS	2.0
1	B	307	ALA	2.0
1	B	242	PRO	2.0
1	A	367	LEU	2.0
1	B	300	MET	2.0
1	B	301	MET	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](#)

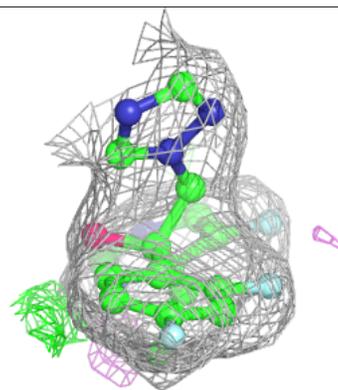
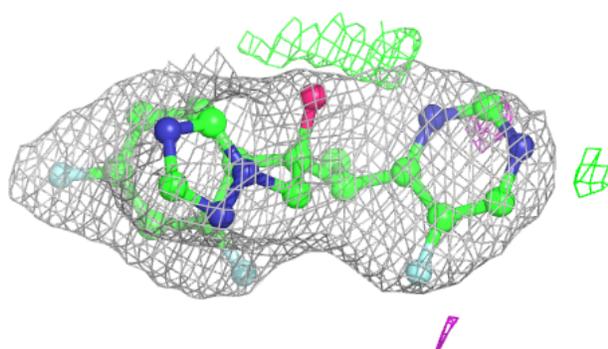
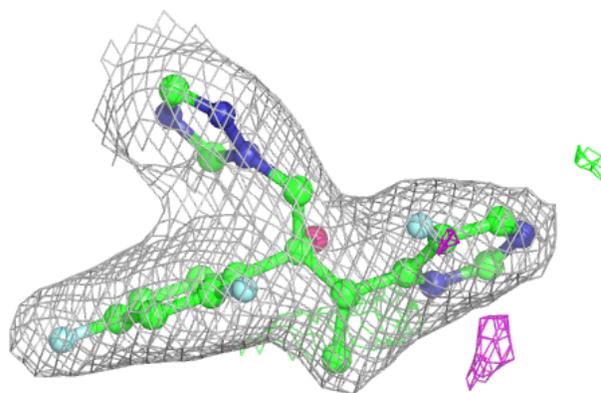
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	VOR	A	590	25/25	0.93	0.30	48,62,73,80	0
3	VOR	B	590	25/25	0.95	0.19	59,69,99,106	0
2	HEM	B	580	43/43	0.96	0.19	49,64,74,77	0
2	HEM	A	580	43/43	0.98	0.23	41,52,75,85	0

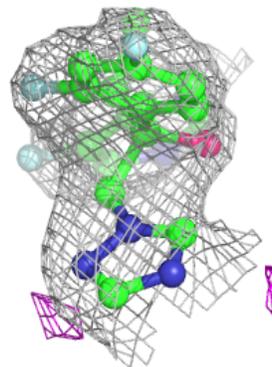
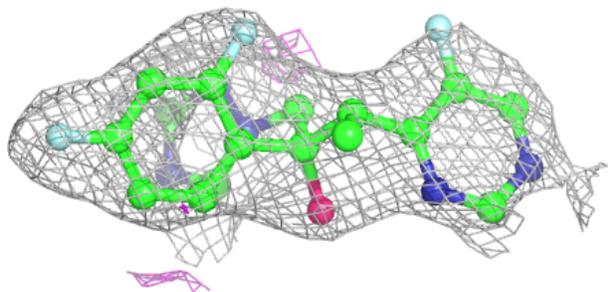
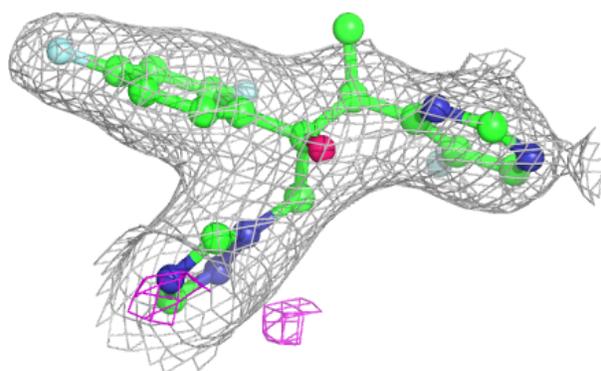
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VOR A 590:

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

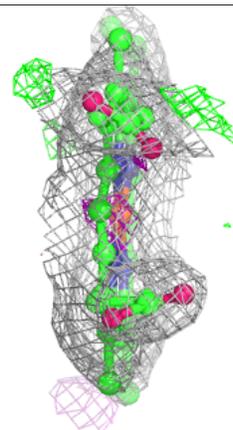
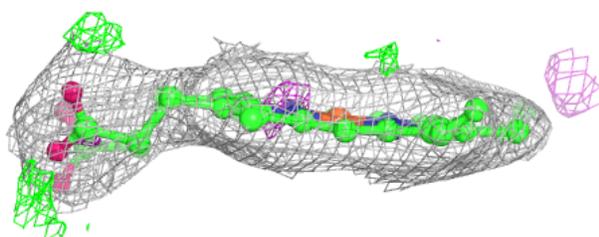
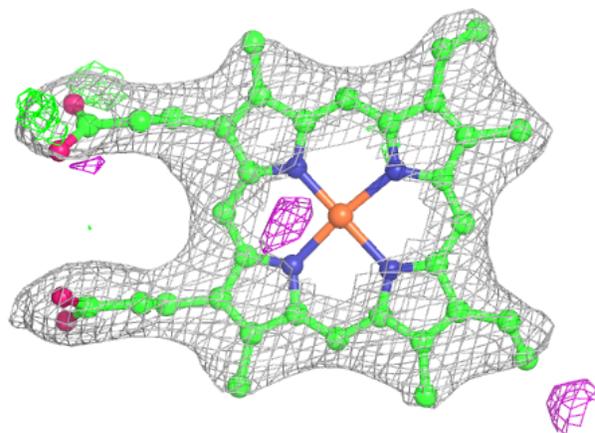
**Electron density around VOR B 590:**

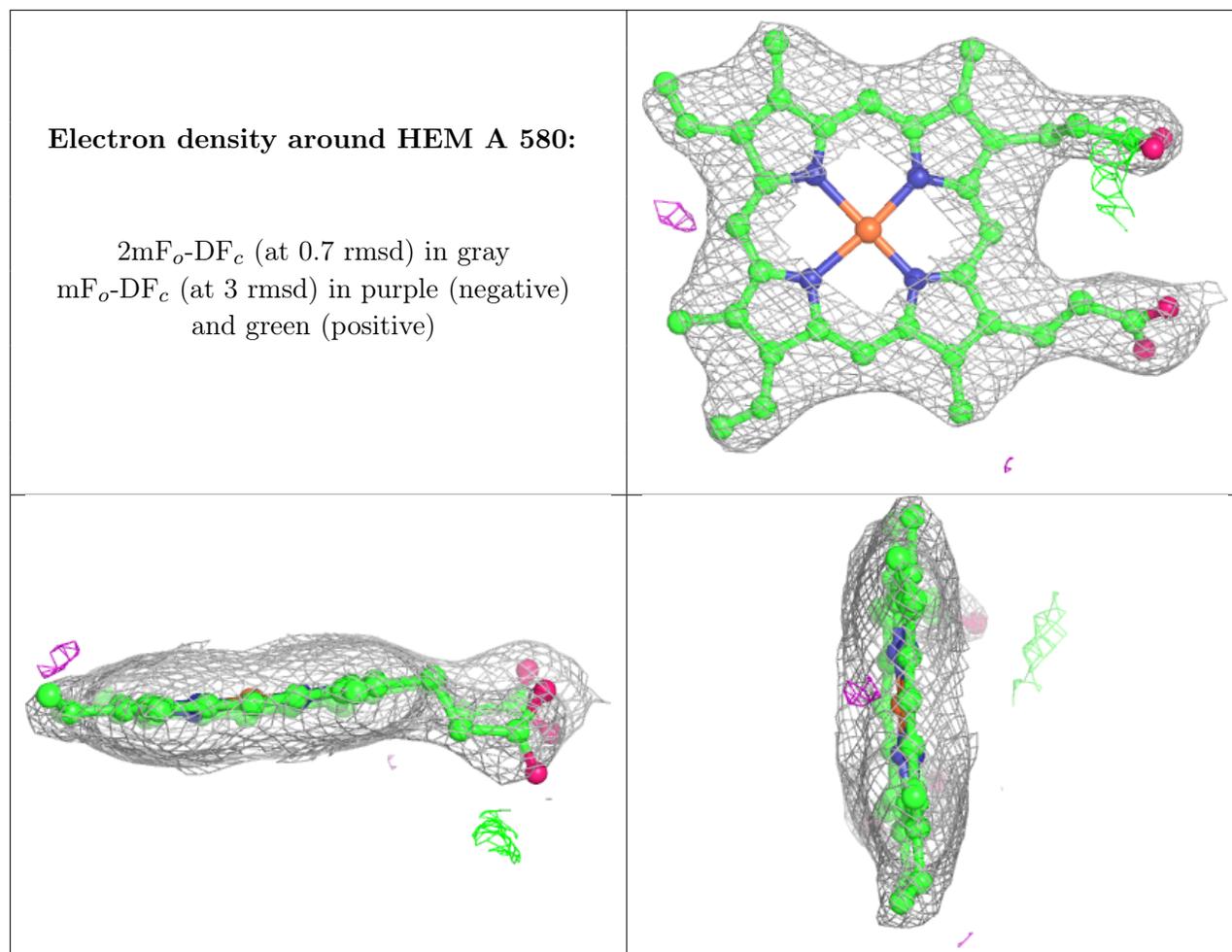
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 580:

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





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

There are no such residues in this entry.