



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:54 AM EDT

PDB ID : 1DT6 / pdb_00001dt6
Title : STRUCTURE OF MAMMALIAN CYTOCHROME P450 2C5
Authors : Williams, P.A.; Cosme, J.; Sridhar, V.; Johnson, E.F.; McRee, D.E.
Deposited on : 2000-01-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

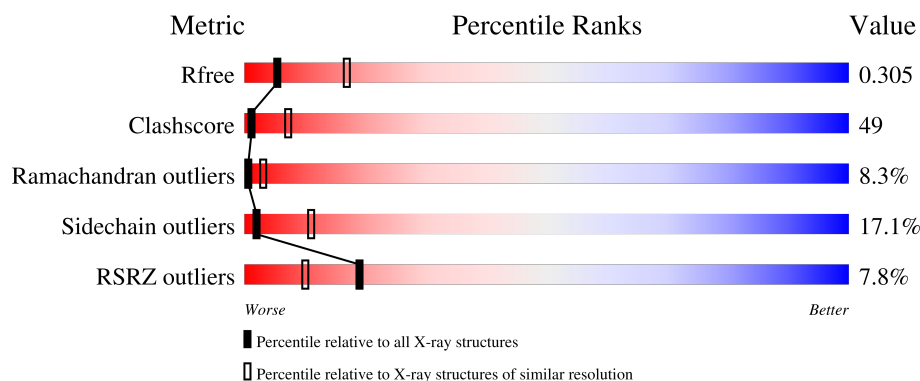
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	473	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3648 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 CYTOCHROME P450 2C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3589	2309	603	655	22			

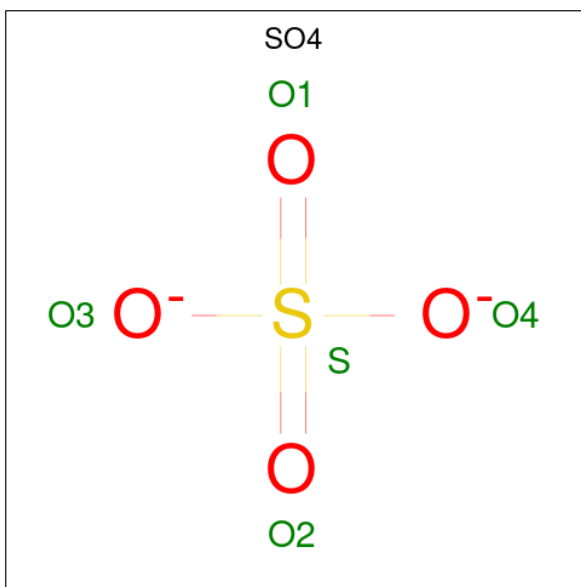
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P00179
A	20	ALA	-	expression tag	UNP P00179
A	22	LYS	GLN	engineered mutation	UNP P00179
A	23	THR	ASN	engineered mutation	UNP P00179
A	25	SER	GLY	engineered mutation	UNP P00179
A	26	LYS	ARG	engineered mutation	UNP P00179
A	97	ARG	THR	engineered mutation	UNP P00179
A	202	HIS	ASN	engineered mutation	UNP P00179
A	206	GLU	ARG	engineered mutation	UNP P00179
A	207	LEU	ILE	engineered mutation	UNP P00179
A	209	GLY	SER	engineered mutation	UNP P00179
A	210	THR	SER	engineered mutation	UNP P00179
A	252	GLN	GLU	engineered mutation	UNP P00179
A	488	HIS	-	expression tag	UNP P00179
A	489	HIS	-	expression tag	UNP P00179
A	490	HIS	-	expression tag	UNP P00179
A	491	HIS	-	expression tag	UNP P00179

- Molecule 2 is SAMARIUM (III) ION (CCD ID: SM) (formula: Sm).

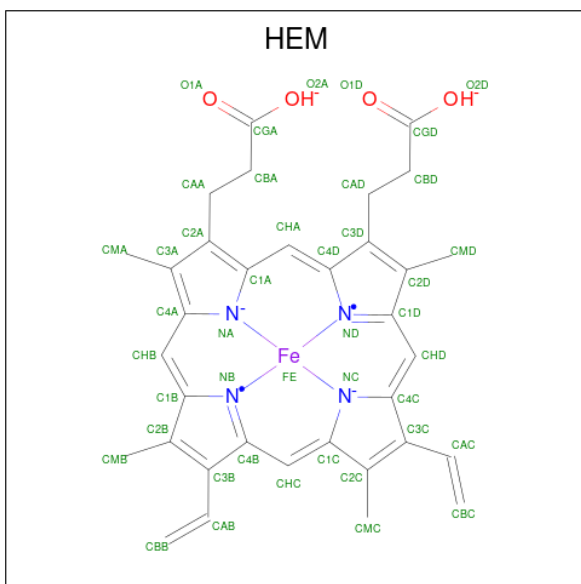
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Sm	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

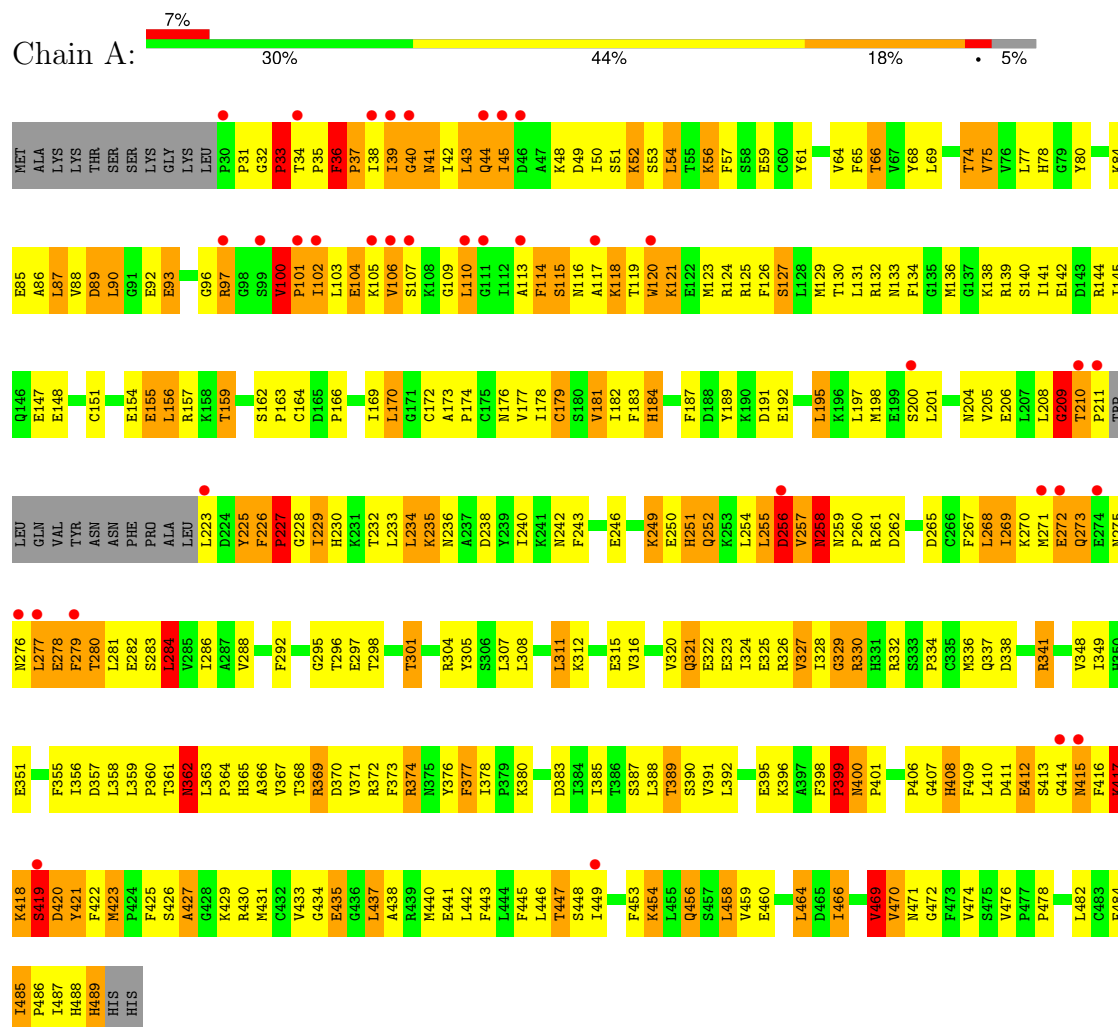


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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: CYTOCHROME P450 2C5



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.70Å 132.00Å 172.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.04	Depositor EDS
% Data completeness (in resolution range)	93.2 (25.00-3.00) 96.8 (25.00-3.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.05Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.238 , 0.313 0.234 , 0.305	Depositor DCC
R_{free} test set	809 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3648	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEM, SM

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	0.50	0/3672	1.21	45/4965 (0.9%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	N-CA-C	-14.04	93.31	114.64
1	A	34	THR	N-CA-C	13.48	120.26	108.13
1	A	278	GLU	N-CA-C	-10.44	100.68	113.41
1	A	429	LYS	N-CA-C	-9.68	100.33	113.30
1	A	48	LYS	N-CA-C	-8.92	101.71	112.59
1	A	419	SER	N-CA-C	8.91	129.77	110.80
1	A	56	LYS	N-CA-C	-8.81	101.65	111.07
1	A	256	ASP	N-CA-C	8.67	122.18	109.69
1	A	322	GLU	N-CA-C	-8.45	101.76	110.97
1	A	257	VAL	N-CA-C	-8.33	96.96	108.12
1	A	361	THR	N-CA-C	-7.99	96.20	109.07
1	A	421	TYR	N-CA-C	-7.89	103.73	112.72
1	A	469	VAL	N-CA-C	-7.78	97.07	108.89
1	A	454	LYS	N-CA-C	-7.54	97.45	109.59
1	A	156	LEU	N-CA-C	-6.65	104.11	111.82
1	A	138	LYS	N-CA-C	6.62	119.32	111.71
1	A	100	VAL	N-CA-C	6.55	123.03	108.88
1	A	400	ASN	CA-C-N	6.54	126.47	119.28
1	A	400	ASN	C-N-CA	6.54	126.47	119.28
1	A	54	LEU	N-CA-C	-6.49	104.62	112.54
1	A	414	GLY	N-CA-C	-6.43	102.32	112.61
1	A	326	ARG	N-CA-C	6.13	117.97	111.28
1	A	78	HIS	N-CA-C	6.07	121.00	112.93
1	A	209	GLY	N-CA-C	5.96	127.29	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	TYR	N-CA-C	-5.61	105.24	111.36
1	A	179	CYS	N-CA-C	-5.58	105.28	111.36
1	A	423	MET	CA-C-N	-5.56	113.95	119.56
1	A	423	MET	C-N-CA	-5.56	113.95	119.56
1	A	89	ASP	N-CA-C	5.49	116.94	111.07
1	A	87	LEU	N-CA-C	5.49	117.97	111.33
1	A	279	PHE	N-CA-C	-5.47	101.94	110.10
1	A	458	LEU	N-CA-C	-5.38	105.00	113.02
1	A	273	GLN	N-CA-C	-5.31	104.58	111.74
1	A	485	ILE	CA-C-N	5.30	125.22	119.76
1	A	485	ILE	C-N-CA	5.30	125.22	119.76
1	A	40	GLY	N-CA-C	-5.30	107.91	115.64
1	A	104	GLU	N-CA-C	5.29	119.49	112.72
1	A	116	ASN	N-CA-C	5.24	117.82	109.96
1	A	453	PHE	N-CA-C	5.21	117.31	109.23
1	A	415	ASN	N-CA-C	-5.18	102.82	110.48
1	A	355	PHE	N-CA-C	5.16	116.99	111.36
1	A	311	LEU	N-CA-C	-5.13	105.39	111.69
1	A	283	SER	N-CA-C	-5.11	105.79	111.36
1	A	396	LYS	N-CA-C	-5.06	106.27	112.90
1	A	257	VAL	CB-CA-C	-5.01	105.89	111.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3589	0	3613	356	1
2	A	1	0	0	0	0
3	A	15	0	0	0	0
4	A	43	0	30	8	0
All	All	3648	0	3643	356	1

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 49.

All (356) 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:225:TYR:HB2	1:A:227:PRO:HB3	1.39	1.05
1:A:417:LYS:HG3	1:A:418:LYS:H	1.30	0.97
1:A:362:ASN:H	1:A:362:ASN:HD22	1.01	0.94
1:A:277:LEU:HG	1:A:278:GLU:H	1.31	0.92
1:A:276:ASN:O	1:A:277:LEU:HB3	1.69	0.91
1:A:417:LYS:O	1:A:418:LYS:HG3	1.72	0.90
1:A:362:ASN:HD22	1:A:362:ASN:N	1.68	0.90
1:A:330:ARG:HH12	1:A:489:HIS:HB2	1.36	0.88
1:A:51:SER:OG	1:A:389:THR:HG21	1.74	0.88
1:A:117:ALA:HA	1:A:120:TRP:HB3	1.55	0.87
1:A:38:ILE:O	1:A:39:ILE:HG12	1.75	0.87
1:A:362:ASN:H	1:A:362:ASN:ND2	1.72	0.86
1:A:100:VAL:HG23	1:A:101:PRO:HD3	1.56	0.86
1:A:411:ASP:OD1	1:A:416:PHE:HB2	1.76	0.85
1:A:256:ASP:HB3	1:A:259:ASN:HB3	1.59	0.84
1:A:443:PHE:O	1:A:447:THR:HB	1.76	0.84
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.60	0.82
1:A:114:PHE:O	1:A:115:SER:HB2	1.82	0.80
1:A:362:ASN:HB2	4:A:501:HEM:HBA1	1.64	0.80
1:A:54:LEU:HD11	1:A:385:ILE:HD11	1.63	0.79
1:A:369:ARG:HG3	1:A:370:ASP:H	1.48	0.79
1:A:399:PRO:O	1:A:401:PRO:HD3	1.84	0.78
1:A:267:PHE:O	1:A:270:LYS:HB2	1.84	0.78
1:A:204:ASN:HD21	1:A:236:ASN:HB2	1.49	0.78
1:A:142:GLU:HB2	1:A:440:MET:HE1	1.64	0.78
1:A:42:ILE:C	1:A:44:GLN:H	1.91	0.76
1:A:97:ARG:N	1:A:97:ARG:NE	2.34	0.75
1:A:44:GLN:HG2	1:A:45:ILE:HG22	1.68	0.75
1:A:357:ASP:OD1	1:A:389:THR:HB	1.87	0.74
1:A:93:GLU:HG2	1:A:371:VAL:HG12	1.69	0.74
1:A:368:THR:O	1:A:369:ARG:HB2	1.85	0.74
1:A:376:TYR:O	1:A:377:PHE:HB3	1.88	0.74
1:A:311:LEU:HD11	1:A:482:LEU:HD13	1.69	0.73
1:A:341:ARG:HH21	1:A:341:ARG:HG2	1.52	0.73
1:A:258:ASN:C	1:A:260:PRO:HD3	2.12	0.73
1:A:155:GLU:HB2	1:A:169:ILE:HD11	1.71	0.73
1:A:156:LEU:O	1:A:159:THR:HB	1.88	0.73
1:A:210:THR:OG1	1:A:472:GLY:HA2	1.89	0.73
1:A:330:ARG:NH1	1:A:489:HIS:HB2	2.03	0.73
1:A:44:GLN:HG2	1:A:45:ILE:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HA	1:A:380:LYS:HD3	1.68	0.73
1:A:42:ILE:HG22	1:A:68:TYR:O	1.88	0.73
1:A:64:VAL:HG21	1:A:373:PHE:HE2	1.54	0.72
1:A:105:LYS:HE2	1:A:106:VAL:HG13	1.72	0.72
1:A:118:LYS:HG3	1:A:119:THR:N	2.03	0.72
1:A:45:ILE:HG23	1:A:57:PHE:HZ	1.54	0.72
1:A:369:ARG:HH11	1:A:380:LYS:NZ	1.87	0.72
1:A:312:LYS:HE2	1:A:466:ILE:HD12	1.70	0.71
1:A:145:ILE:HD12	1:A:441:GLU:HG2	1.72	0.71
1:A:85:GLU:O	1:A:89:ASP:HB2	1.91	0.70
1:A:192:GLU:HA	1:A:195:LEU:HD12	1.73	0.70
1:A:226:PHE:N	1:A:227:PRO:HA	2.06	0.70
1:A:69:LEU:HG	1:A:74:THR:HG21	1.74	0.70
1:A:42:ILE:HG21	1:A:68:TYR:H	1.55	0.70
1:A:437:LEU:O	1:A:441:GLU:HG3	1.93	0.69
1:A:154:GLU:O	1:A:157:ARG:HB2	1.91	0.69
1:A:334:PRO:HG2	1:A:447:THR:CG2	2.22	0.69
1:A:100:VAL:CG2	1:A:101:PRO:HD3	2.22	0.69
1:A:395:GLU:HA	1:A:401:PRO:HG3	1.74	0.69
1:A:144:ARG:HH11	1:A:181:VAL:HA	1.59	0.68
1:A:277:LEU:HG	1:A:278:GLU:N	2.08	0.67
1:A:391:VAL:HG11	1:A:423:MET:HE3	1.76	0.67
1:A:32:GLY:O	1:A:66:THR:HG23	1.95	0.67
1:A:126:PHE:O	1:A:130:THR:HG23	1.94	0.66
1:A:133:ASN:HD21	1:A:142:GLU:H	1.41	0.66
1:A:102:ILE:HD11	1:A:208:LEU:HD13	1.78	0.66
1:A:41:ASN:CB	1:A:43:LEU:HD13	2.24	0.66
1:A:225:TYR:CB	1:A:227:PRO:HB3	2.21	0.66
1:A:201:LEU:HD23	1:A:240:ILE:HD13	1.77	0.66
1:A:336:MET:HG3	1:A:440:MET:HE3	1.77	0.66
1:A:38:ILE:O	1:A:39:ILE:HG23	1.95	0.66
1:A:210:THR:HG22	1:A:211:PRO:HD2	1.77	0.66
1:A:49:ASP:OD2	1:A:52:LYS:HB2	1.96	0.65
1:A:469:VAL:HG22	1:A:476:VAL:HG23	1.77	0.65
1:A:142:GLU:HB2	1:A:440:MET:CE	2.25	0.65
1:A:297:GLU:O	1:A:301:THR:HG22	1.97	0.65
1:A:278:GLU:O	1:A:280:THR:HG23	1.96	0.65
1:A:151:CYS:O	1:A:155:GLU:HG2	1.96	0.64
1:A:39:ILE:HG13	1:A:39:ILE:O	1.96	0.64
1:A:358:LEU:O	1:A:359:LEU:HD12	1.98	0.64
1:A:42:ILE:C	1:A:44:GLN:N	2.52	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HD21	1:A:484:PHE:CE1	2.33	0.64
1:A:96:GLY:HA2	1:A:97:ARG:NH1	2.14	0.63
1:A:363:LEU:HG	4:A:501:HEM:HAA2	1.79	0.63
1:A:45:ILE:HG23	1:A:57:PHE:CZ	2.33	0.63
1:A:341:ARG:HG2	1:A:341:ARG:NH2	2.13	0.63
1:A:410:LEU:HD22	1:A:415:ASN:HB3	1.79	0.63
1:A:351:GLU:OE2	1:A:408:HIS:HD2	1.80	0.63
1:A:43:LEU:H	1:A:43:LEU:CD1	2.12	0.62
1:A:204:ASN:HD21	1:A:236:ASN:CB	2.12	0.62
1:A:254:LEU:O	1:A:254:LEU:HD12	1.99	0.62
1:A:170:LEU:HD23	1:A:304:ARG:HA	1.82	0.62
1:A:204:ASN:O	1:A:208:LEU:HG	2.00	0.62
1:A:256:ASP:CB	1:A:259:ASN:HB3	2.29	0.62
1:A:129:MET:O	1:A:132:ARG:HG3	2.00	0.62
1:A:32:GLY:HA2	1:A:376:TYR:CE1	2.35	0.61
1:A:469:VAL:HG22	1:A:476:VAL:CG2	2.30	0.61
1:A:330:ARG:HH12	1:A:489:HIS:CB	2.11	0.61
1:A:103:LEU:HD22	1:A:109:GLY:HA2	1.82	0.61
1:A:235:LYS:HA	1:A:235:LYS:HE2	1.81	0.61
1:A:427:ALA:HA	1:A:431:MET:HG3	1.82	0.60
1:A:172:CYS:SG	1:A:198:MET:HE1	2.42	0.60
1:A:226:PHE:N	1:A:227:PRO:CA	2.64	0.60
1:A:100:VAL:HG23	1:A:101:PRO:CD	2.28	0.59
1:A:417:LYS:HG3	1:A:418:LYS:N	2.06	0.59
1:A:456:GLN:HB3	1:A:485:ILE:HD12	1.83	0.59
1:A:33:PRO:HD3	1:A:376:TYR:HE1	1.66	0.59
1:A:114:PHE:O	1:A:115:SER:CB	2.48	0.59
1:A:64:VAL:HG22	1:A:77:LEU:HD23	1.83	0.59
1:A:257:VAL:O	1:A:259:ASN:N	2.36	0.59
1:A:373:PHE:O	1:A:376:TYR:HB2	2.02	0.59
1:A:418:LYS:O	1:A:419:SER:HB3	2.03	0.59
1:A:66:THR:HA	1:A:75:VAL:HA	1.85	0.59
1:A:277:LEU:CG	1:A:278:GLU:H	2.06	0.59
1:A:101:PRO:O	1:A:103:LEU:N	2.36	0.58
1:A:183:PHE:O	1:A:184:HIS:CB	2.52	0.58
1:A:223:LEU:HD22	1:A:225:TYR:OH	2.04	0.58
1:A:85:GLU:OE2	1:A:374:ARG:HD3	2.03	0.58
1:A:267:PHE:CD2	1:A:279:PHE:HD1	2.22	0.58
1:A:470:VAL:O	1:A:472:GLY:N	2.37	0.58
1:A:295:GLY:HA2	4:A:501:HEM:C2C	2.38	0.58
1:A:105:LYS:HE2	1:A:106:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:HG3	1:A:189:TYR:CE1	2.39	0.57
1:A:257:VAL:O	1:A:258:ASN:C	2.47	0.57
1:A:415:ASN:O	1:A:416:PHE:CD2	2.58	0.57
1:A:417:LYS:NZ	1:A:417:LYS:HA	2.19	0.57
1:A:369:ARG:HH11	1:A:380:LYS:HZ1	1.52	0.56
1:A:97:ARG:HA	1:A:364:PRO:O	2.05	0.56
1:A:210:THR:HG22	1:A:211:PRO:CD	2.34	0.56
1:A:399:PRO:O	1:A:401:PRO:CD	2.51	0.56
1:A:267:PHE:CE2	1:A:284:LEU:HB2	2.41	0.56
1:A:178:ILE:HD11	1:A:295:GLY:HA3	1.88	0.56
1:A:267:PHE:CD2	1:A:279:PHE:CD1	2.93	0.56
1:A:227:PRO:C	1:A:229:ILE:N	2.63	0.56
1:A:454:LYS:HG3	1:A:487:ILE:HG12	1.88	0.56
1:A:41:ASN:HB2	1:A:43:LEU:HD13	1.87	0.55
1:A:358:LEU:C	1:A:359:LEU:HD12	2.32	0.55
1:A:38:ILE:O	1:A:39:ILE:CG1	2.52	0.55
1:A:96:GLY:HA3	1:A:366:ALA:O	2.07	0.55
1:A:110:LEU:HB3	1:A:119:THR:HG21	1.87	0.55
1:A:417:LYS:HA	1:A:417:LYS:HZ3	1.71	0.55
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.72	0.55
1:A:223:LEU:HB3	1:A:225:TYR:OH	2.07	0.55
1:A:369:ARG:HH11	1:A:380:LYS:HZ3	1.55	0.55
1:A:226:PHE:H	1:A:227:PRO:HA	1.67	0.55
1:A:52:LYS:HD2	1:A:56:LYS:HE3	1.90	0.54
1:A:260:PRO:HB3	1:A:265:ASP:HB3	1.89	0.54
1:A:434:GLY:O	1:A:435:GLU:C	2.49	0.54
1:A:33:PRO:HD3	1:A:376:TYR:CE1	2.42	0.54
1:A:308:LEU:HD21	1:A:466:ILE:HA	1.90	0.53
1:A:66:THR:HG22	1:A:75:VAL:HB	1.90	0.53
1:A:105:LYS:HE2	1:A:106:VAL:HG22	1.90	0.53
1:A:242:ASN:O	1:A:243:PHE:C	2.51	0.53
1:A:166:PRO:HG3	1:A:482:LEU:CD2	2.38	0.53
1:A:228:GLY:O	1:A:232:THR:HG23	2.09	0.53
1:A:166:PRO:O	1:A:170:LEU:HB2	2.09	0.53
1:A:166:PRO:HG3	1:A:482:LEU:HD22	1.90	0.53
1:A:259:ASN:N	1:A:260:PRO:HD3	2.21	0.53
1:A:292:PHE:O	1:A:296:THR:HG22	2.08	0.53
1:A:315:GLU:HG2	1:A:316:VAL:N	2.24	0.53
1:A:320:VAL:O	1:A:324:ILE:HG13	2.09	0.53
1:A:96:GLY:O	1:A:365:HIS:HA	2.09	0.53
1:A:311:LEU:HD11	1:A:482:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:SD	1:A:262:ASP:HA	2.50	0.52
1:A:358:LEU:O	1:A:474:VAL:HA	2.10	0.52
1:A:369:ARG:HA	1:A:380:LYS:HB2	1.93	0.51
1:A:49:ASP:CG	1:A:52:LYS:HB2	2.35	0.51
1:A:369:ARG:O	1:A:380:LYS:HA	2.10	0.51
1:A:425:PHE:CE2	1:A:435:GLU:HA	2.45	0.51
1:A:139:ARG:NH2	1:A:147:GLU:OE1	2.39	0.51
1:A:201:LEU:O	1:A:205:VAL:HG23	2.11	0.51
1:A:177:VAL:HG21	1:A:441:GLU:OE1	2.10	0.51
1:A:232:THR:O	1:A:235:LYS:HB3	2.10	0.51
1:A:442:LEU:O	1:A:446:LEU:HB2	2.11	0.51
1:A:296:THR:HG23	1:A:297:GLU:N	2.24	0.51
1:A:249:LYS:NZ	1:A:252:GLN:HE22	2.09	0.51
1:A:323:GLU:O	1:A:327:VAL:HG13	2.10	0.51
1:A:210:THR:N	1:A:472:GLY:CA	2.74	0.50
1:A:157:ARG:C	1:A:159:THR:H	2.19	0.50
1:A:261:ARG:O	1:A:262:ASP:HB3	2.10	0.50
1:A:362:ASN:N	1:A:362:ASN:ND2	2.40	0.50
1:A:260:PRO:HG3	1:A:269:ILE:HD13	1.94	0.50
1:A:369:ARG:NH1	1:A:380:LYS:HZ1	2.09	0.50
1:A:298:THR:HG22	1:A:358:LEU:HD21	1.92	0.50
1:A:466:ILE:HD13	1:A:466:ILE:H	1.77	0.50
1:A:133:ASN:ND2	1:A:140:SER:HB2	2.26	0.50
1:A:369:ARG:CA	1:A:380:LYS:HD3	2.42	0.50
1:A:170:LEU:HD23	1:A:304:ARG:CA	2.42	0.49
1:A:376:TYR:O	1:A:377:PHE:CB	2.58	0.49
1:A:166:PRO:HB2	1:A:170:LEU:HD22	1.95	0.49
1:A:277:LEU:CG	1:A:278:GLU:N	2.71	0.49
1:A:120:TRP:O	1:A:121:LYS:C	2.55	0.49
1:A:417:LYS:CG	1:A:418:LYS:H	2.13	0.49
1:A:140:SER:O	1:A:144:ARG:HG3	2.13	0.49
1:A:210:THR:CG2	1:A:211:PRO:HD2	2.40	0.49
1:A:426:SER:HB2	4:A:501:HEM:HBA2	1.94	0.49
1:A:307:LEU:HD21	1:A:449:ILE:HD11	1.94	0.49
1:A:459:VAL:O	1:A:460:GLU:C	2.55	0.49
1:A:69:LEU:HG	1:A:74:THR:CG2	2.42	0.49
1:A:84:LYS:HE3	1:A:88:VAL:HG21	1.95	0.49
1:A:269:ILE:O	1:A:269:ILE:HG13	2.11	0.49
1:A:201:LEU:HD23	1:A:240:ILE:CD1	2.42	0.48
1:A:369:ARG:HG3	1:A:370:ASP:N	2.25	0.48
1:A:415:ASN:O	1:A:416:PHE:CG	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:CD1	1:A:43:LEU:N	2.77	0.48
1:A:97:ARG:CZ	1:A:97:ARG:H	2.27	0.48
1:A:125:ARG:HD3	1:A:125:ARG:C	2.38	0.48
1:A:273:GLN:NE2	1:A:277:LEU:HD13	2.29	0.48
1:A:368:THR:O	1:A:369:ARG:CB	2.55	0.48
1:A:411:ASP:C	1:A:413:SER:H	2.21	0.48
1:A:398:PHE:O	1:A:399:PRO:C	2.57	0.48
1:A:133:ASN:ND2	1:A:142:GLU:H	2.10	0.48
1:A:334:PRO:HG2	1:A:447:THR:HG22	1.96	0.48
1:A:97:ARG:N	1:A:97:ARG:CZ	2.77	0.48
1:A:141:ILE:O	1:A:145:ILE:HG12	2.14	0.48
1:A:157:ARG:HG2	1:A:157:ARG:NH1	2.29	0.48
1:A:371:VAL:HG23	1:A:378:ILE:HB	1.95	0.48
1:A:307:LEU:HD21	1:A:449:ILE:CD1	2.44	0.48
1:A:41:ASN:HB3	1:A:43:LEU:HD13	1.95	0.48
1:A:43:LEU:HD13	1:A:43:LEU:H	1.77	0.48
1:A:208:LEU:O	1:A:209:GLY:O	2.32	0.48
1:A:42:ILE:HG21	1:A:68:TYR:N	2.25	0.47
1:A:328:ILE:O	1:A:329:GLY:O	2.32	0.47
1:A:42:ILE:O	1:A:42:ILE:HG23	2.15	0.47
1:A:40:GLY:C	1:A:41:ASN:CG	2.83	0.47
1:A:356:ILE:O	1:A:357:ASP:C	2.57	0.47
1:A:387:SER:OG	1:A:390:SER:HB3	2.15	0.47
1:A:183:PHE:O	1:A:184:HIS:HB2	2.14	0.47
1:A:332:ARG:HH22	1:A:338:ASP:CG	2.22	0.47
1:A:84:LYS:CE	1:A:88:VAL:HG21	2.45	0.47
1:A:484:PHE:O	1:A:486:PRO:HD3	2.14	0.47
1:A:77:LEU:HD13	1:A:86:ALA:CB	2.44	0.47
1:A:201:LEU:HD13	1:A:296:THR:HG21	1.97	0.47
1:A:279:PHE:O	1:A:280:THR:HG22	2.14	0.47
1:A:369:ARG:CA	1:A:380:LYS:HB2	2.45	0.47
1:A:109:GLY:C	1:A:110:LEU:HD23	2.40	0.46
1:A:123:MET:HE2	1:A:123:MET:HA	1.98	0.46
1:A:312:LYS:HG2	1:A:466:ILE:HG21	1.97	0.46
1:A:407:GLY:C	1:A:409:PHE:N	2.72	0.46
1:A:151:CYS:O	1:A:155:GLU:CG	2.63	0.46
1:A:332:ARG:NH2	1:A:338:ASP:OD2	2.48	0.46
1:A:64:VAL:HG21	1:A:373:PHE:CE2	2.43	0.46
1:A:176:ASN:HA	1:A:179:CYS:HB2	1.97	0.46
1:A:210:THR:N	1:A:472:GLY:HA3	2.30	0.46
1:A:191:ASP:C	1:A:191:ASP:OD2	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:SER:O	1:A:390:SER:OG	2.30	0.46
1:A:255:LEU:HD12	1:A:269:ILE:CG2	2.46	0.46
1:A:445:PHE:O	1:A:449:ILE:HG23	2.15	0.46
1:A:210:THR:H	1:A:472:GLY:HA2	1.81	0.46
1:A:440:MET:O	1:A:441:GLU:C	2.58	0.46
1:A:144:ARG:NH1	1:A:181:VAL:HA	2.30	0.46
1:A:227:PRO:C	1:A:229:ILE:H	2.23	0.46
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.81	0.46
1:A:105:LYS:O	1:A:107:SER:N	2.49	0.45
1:A:74:THR:HB	1:A:383:ASP:HB2	1.97	0.45
1:A:93:GLU:HG2	1:A:371:VAL:CG1	2.42	0.45
1:A:100:VAL:O	1:A:101:PRO:C	2.59	0.45
1:A:118:LYS:HE2	1:A:119:THR:OG1	2.16	0.45
1:A:246:GLU:O	1:A:250:GLU:HG2	2.16	0.45
1:A:431:MET:HE2	1:A:431:MET:HB3	1.77	0.45
1:A:254:LEU:C	1:A:255:LEU:HD23	2.42	0.45
1:A:411:ASP:O	1:A:413:SER:N	2.42	0.45
1:A:410:LEU:HD22	1:A:415:ASN:CB	2.44	0.45
1:A:35:PRO:O	1:A:36:PHE:C	2.60	0.45
1:A:42:ILE:HB	1:A:68:TYR:HB2	2.00	0.44
1:A:56:LYS:O	1:A:59:GLU:HB2	2.16	0.44
1:A:182:ILE:HG21	1:A:288:VAL:HG13	1.99	0.44
1:A:357:ASP:O	1:A:360:PRO:HD3	2.17	0.44
1:A:105:LYS:HE2	1:A:106:VAL:CG2	2.47	0.44
1:A:411:ASP:C	1:A:411:ASP:OD2	2.60	0.44
1:A:407:GLY:O	1:A:409:PHE:N	2.51	0.44
1:A:227:PRO:O	1:A:230:HIS:N	2.39	0.44
1:A:156:LEU:HD22	1:A:484:PHE:CD2	2.52	0.44
1:A:210:THR:H	1:A:472:GLY:CA	2.30	0.44
1:A:53:SER:HA	1:A:56:LYS:HG3	1.99	0.44
1:A:234:LEU:O	1:A:238:ASP:HB2	2.17	0.44
1:A:349:ILE:CD1	1:A:443:PHE:HA	2.47	0.44
1:A:38:ILE:C	1:A:39:ILE:HG12	2.40	0.44
1:A:61:TYR:CB	1:A:65:PHE:HB3	2.47	0.44
1:A:321:GLN:HE21	1:A:321:GLN:HB2	1.54	0.44
1:A:447:THR:HG22	1:A:448:SER:N	2.32	0.44
1:A:113:ALA:O	1:A:114:PHE:HB2	2.18	0.44
1:A:362:ASN:CB	4:A:501:HEM:HBA1	2.43	0.44
1:A:438:ALA:HB1	4:A:501:HEM:HAB	1.99	0.44
1:A:105:LYS:C	1:A:107:SER:N	2.74	0.43
1:A:179:CYS:HG	1:A:187:PHE:HE1	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HA	1:A:235:LYS:CE	2.46	0.43
1:A:255:LEU:HD23	1:A:255:LEU:N	2.31	0.43
1:A:301:THR:O	1:A:305:TYR:HB2	2.18	0.43
1:A:200:SER:O	1:A:201:LEU:C	2.62	0.43
1:A:210:THR:CG2	1:A:211:PRO:CD	2.96	0.43
1:A:407:GLY:C	1:A:409:PHE:H	2.26	0.43
1:A:446:LEU:O	1:A:449:ILE:HG12	2.18	0.43
1:A:262:ASP:OD2	1:A:262:ASP:C	2.61	0.43
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.83	0.43
1:A:351:GLU:OE2	1:A:408:HIS:CD2	2.66	0.43
1:A:74:THR:HA	1:A:383:ASP:O	2.19	0.43
1:A:177:VAL:O	1:A:181:VAL:HG13	2.19	0.43
1:A:38:ILE:O	1:A:39:ILE:CG2	2.64	0.43
1:A:225:TYR:CD1	1:A:225:TYR:N	2.85	0.43
1:A:282:GLU:O	1:A:286:ILE:HG13	2.19	0.43
1:A:54:LEU:HD11	1:A:385:ILE:CD1	2.42	0.43
1:A:105:LYS:CE	1:A:106:VAL:HG22	2.48	0.43
1:A:110:LEU:O	1:A:286:ILE:HG21	2.19	0.43
1:A:229:ILE:O	1:A:233:LEU:HG	2.19	0.42
1:A:369:ARG:O	1:A:380:LYS:CA	2.66	0.42
1:A:312:LYS:HD3	1:A:464:LEU:CD1	2.49	0.42
1:A:417:LYS:CG	1:A:418:LYS:N	2.77	0.42
1:A:334:PRO:HG2	1:A:447:THR:HG23	1.99	0.42
1:A:458:LEU:C	1:A:459:VAL:HG23	2.44	0.42
1:A:134:PHE:CZ	1:A:140:SER:HB3	2.54	0.42
1:A:84:LYS:HD2	1:A:88:VAL:HG21	2.01	0.42
1:A:36:PHE:HA	1:A:37:PRO:HD2	1.86	0.42
1:A:42:ILE:CG2	1:A:68:TYR:O	2.62	0.42
1:A:113:ALA:HB2	4:A:501:HEM:HAD1	2.02	0.42
1:A:117:ALA:O	1:A:118:LYS:C	2.61	0.42
1:A:398:PHE:CE1	1:A:421:TYR:HB2	2.55	0.42
1:A:31:PRO:HB2	1:A:66:THR:HG21	2.02	0.42
1:A:148:GLU:OE1	1:A:176:ASN:HB3	2.20	0.42
1:A:482:LEU:HD21	1:A:484:PHE:CZ	2.54	0.42
1:A:210:THR:HG22	1:A:211:PRO:N	2.35	0.41
1:A:210:THR:N	1:A:472:GLY:HA2	2.35	0.41
1:A:437:LEU:HD12	1:A:437:LEU:C	2.44	0.41
1:A:348:VAL:HG22	1:A:406:PRO:CG	2.51	0.41
1:A:157:ARG:C	1:A:159:THR:N	2.76	0.41
1:A:420:ASP:C	1:A:422:PHE:H	2.27	0.41
1:A:423:MET:HG2	1:A:427:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:O	1:A:268:LEU:C	2.63	0.41
1:A:388:LEU:O	1:A:389:THR:C	2.61	0.41
1:A:412:GLU:O	1:A:412:GLU:HG3	2.20	0.41
1:A:40:GLY:O	1:A:41:ASN:CB	2.68	0.41
1:A:362:ASN:HB2	1:A:363:LEU:H	1.65	0.41
1:A:43:LEU:N	1:A:43:LEU:HD12	2.36	0.41
1:A:105:LYS:HB2	1:A:234:LEU:CD2	2.50	0.41
1:A:296:THR:CG2	1:A:297:GLU:N	2.84	0.41
1:A:312:LYS:HD3	1:A:464:LEU:HD12	2.02	0.41
1:A:90:LEU:N	1:A:90:LEU:CD1	2.84	0.41
1:A:183:PHE:O	1:A:251:HIS:CE1	2.73	0.41
1:A:192:GLU:CA	1:A:195:LEU:HD12	2.46	0.41
1:A:272:GLU:O	1:A:273:GLN:HB3	2.20	0.41
1:A:433:VAL:CG2	4:A:501:HEM:HBD2	2.51	0.41
1:A:33:PRO:HB2	1:A:61:TYR:HD1	1.85	0.41
1:A:127:SER:O	1:A:131:LEU:HB2	2.21	0.41
1:A:170:LEU:CD2	1:A:304:ARG:HA	2.49	0.40
1:A:61:TYR:HB3	1:A:65:PHE:HB3	2.01	0.40
1:A:97:ARG:N	1:A:97:ARG:CD	2.84	0.40
1:A:204:ASN:ND2	1:A:236:ASN:CB	2.81	0.40
1:A:227:PRO:O	1:A:229:ILE:N	2.55	0.40
1:A:162:SER:OG	1:A:163:PRO:HD2	2.21	0.40
1:A:425:PHE:O	1:A:431:MET:HG2	2.22	0.40
1:A:93:GLU:HB3	1:A:371:VAL:HG11	2.04	0.40
1:A:279:PHE:C	1:A:280:THR:CG2	2.93	0.40
1:A:370:ASP:O	1:A:371:VAL:HG13	2.20	0.40
1:A:42:ILE:O	1:A:44:GLN:N	2.54	0.40
1:A:225:TYR:O	1:A:225:TYR:HD1	2.05	0.40
1:A:427:ALA:CA	1:A:431:MET:HG3	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:CD1	1:A:229:ILE:CD1[2_555]	1.75	0.45

5.3 Torsion angles

5.3.1 Protein backbone

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	445/473 (94%)	325 (73%)	83 (19%)	37 (8%)	0 3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	39	ILE
1	A	102	ILE
1	A	115	SER
1	A	209	GLY
1	A	258	ASN
1	A	275	ASN
1	A	277	LEU
1	A	369	ARG
1	A	399	PRO
1	A	417	LYS
1	A	471	ASN
1	A	33	PRO
1	A	120	TRP
1	A	210	THR
1	A	329	GLY
1	A	362	ASN
1	A	412	GLU
1	A	418	LYS
1	A	37	PRO
1	A	101	PRO
1	A	184	HIS
1	A	377	PHE
1	A	420	ASP
1	A	100	VAL
1	A	121	LYS
1	A	408	HIS
1	A	114	PHE

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	400	ASN
1	A	427	ALA
1	A	419	SER
1	A	435	GLU
1	A	478	PRO
1	A	269	ILE
1	A	106	VAL
1	A	227	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	404/425 (95%)	335 (83%)	69 (17%)	2 11

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	A	36	PHE
1	A	41	ASN
1	A	43	LEU
1	A	44	GLN
1	A	45	ILE
1	A	50	ILE
1	A	52	LYS
1	A	66	THR
1	A	74	THR
1	A	75	VAL
1	A	87	LEU
1	A	90	LEU
1	A	92	GLU
1	A	93	GLU
1	A	97	ARG
1	A	104	GLU

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Mol	Chain	Res	Type
1	A	110	LEU
1	A	118	LYS
1	A	127	SER
1	A	155	GLU
1	A	159	THR
1	A	164	CYS
1	A	170	LEU
1	A	181	VAL
1	A	195	LEU
1	A	197	LEU
1	A	206	GLU
1	A	225	TYR
1	A	226	PHE
1	A	227	PRO
1	A	229	ILE
1	A	234	LEU
1	A	235	LYS
1	A	249	LYS
1	A	251	HIS
1	A	252	GLN
1	A	255	LEU
1	A	256	ASP
1	A	258	ASN
1	A	268	LEU
1	A	271	MET
1	A	272	GLU
1	A	280	THR
1	A	284	LEU
1	A	301	THR
1	A	321	GLN
1	A	325	GLU
1	A	327	VAL
1	A	337	GLN
1	A	341	ARG
1	A	362	ASN
1	A	367	VAL
1	A	372	ARG
1	A	374	ARG
1	A	389	THR
1	A	392	LEU
1	A	399	PRO
1	A	417	LYS

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Mol	Chain	Res	Type
1	A	430	ARG
1	A	437	LEU
1	A	447	THR
1	A	456	GLN
1	A	464	LEU
1	A	466	ILE
1	A	469	VAL
1	A	470	VAL
1	A	488	HIS
1	A	489	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	133	ASN
1	A	184	HIS
1	A	204	ASN
1	A	236	ASN
1	A	242	ASN
1	A	252	GLN
1	A	273	GLN
1	A	321	GLN
1	A	337	GLN
1	A	362	ASN
1	A	408	HIS
1	A	451	GLN
1	A	471	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
3	SO4	A	503	-	4,4,4	0.32	0	6,6,6	0.11	0
4	HEM	A	501	1	50,50,50	2.30	21 (42%)	67,82,82	1.17	5 (7%)
3	SO4	A	505	-	4,4,4	0.33	0	6,6,6	0.15	0
3	SO4	A	504	-	4,4,4	0.38	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	501	1	-	4/14/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HEM	FE-ND	5.25	2.11	1.94
4	A	501	HEM	FE-NC	4.28	2.09	1.95
4	A	501	HEM	C1B-NB	-4.25	1.32	1.40
4	A	501	HEM	FE-NB	4.19	2.07	1.94
4	A	501	HEM	FE-NA	3.83	2.07	1.95
4	A	501	HEM	C4D-ND	-3.72	1.33	1.40
4	A	501	HEM	CBC-CAC	3.21	1.45	1.30
4	A	501	HEM	C3C-C4C	-3.19	1.40	1.46
4	A	501	HEM	C4A-NA	-3.06	1.33	1.39
4	A	501	HEM	CBB-CAB	2.93	1.44	1.30
4	A	501	HEM	C4B-NB	-2.86	1.33	1.38
4	A	501	HEM	C1C-NC	-2.75	1.34	1.39
4	A	501	HEM	C1C-C2C	-2.71	1.40	1.45
4	A	501	HEM	C1A-NA	-2.41	1.35	1.39
4	A	501	HEM	O2D-CGD	-2.39	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HEM	C1D-C2D	-2.35	1.39	1.44
4	A	501	HEM	O2A-CGA	-2.32	1.23	1.30
4	A	501	HEM	C3C-C2C	2.31	1.41	1.37
4	A	501	HEM	CHD-C4C	2.22	1.42	1.38
4	A	501	HEM	C1A-C2A	-2.16	1.40	1.44
4	A	501	HEM	CAA-C2A	2.04	1.56	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	HEM	C4B-C3B-C2B	-2.77	104.73	107.28
4	A	501	HEM	C1C-CHC-C4B	2.39	131.10	126.02
4	A	501	HEM	O2A-CGA-CBA	2.27	121.17	114.00
4	A	501	HEM	C3B-C4B-NB	2.26	111.09	109.47
4	A	501	HEM	CBA-CAA-C2A	2.18	118.56	112.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	HEM	C1A-C2A-CAA-CBA
4	A	501	HEM	C3A-C2A-CAA-CBA
4	A	501	HEM	C2A-CAA-CBA-CGA
4	A	501	HEM	C2C-C3C-CAC-CBC

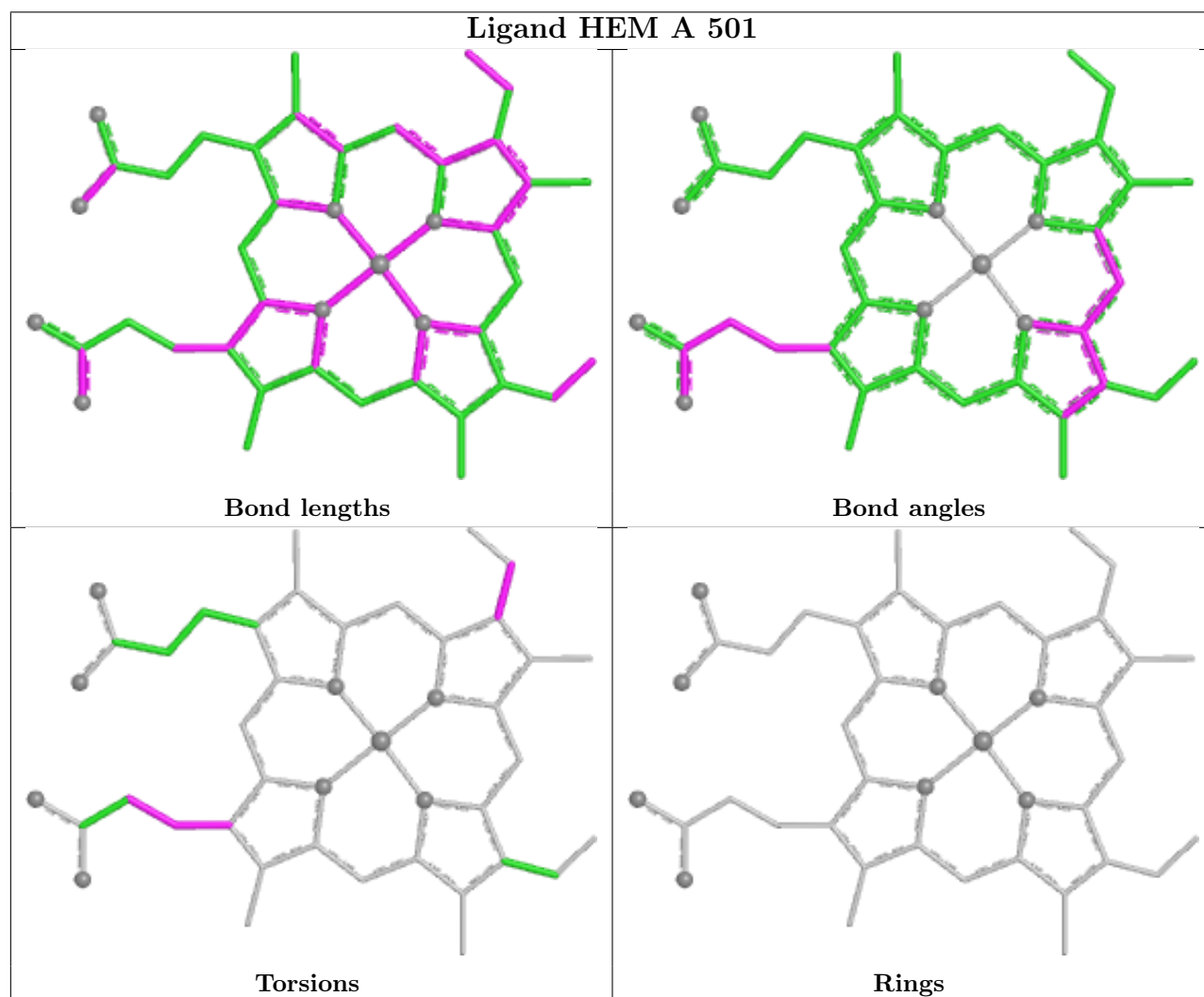
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HEM	8	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	449/473 (94%)	0.31	35 (7%) 19 10	24, 56, 98, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	ASN	5.6
1	A	419	SER	5.1
1	A	223	LEU	4.7
1	A	110	LEU	4.6
1	A	211	PRO	4.5
1	A	30	PRO	3.5
1	A	102	ILE	3.5
1	A	38	ILE	3.5
1	A	277	LEU	3.3
1	A	276	ASN	3.3
1	A	107	SER	3.2
1	A	34	THR	3.2
1	A	117	ALA	3.2
1	A	279	PHE	3.2
1	A	106	VAL	3.1
1	A	111	GLY	3.1
1	A	99	SER	2.9
1	A	44	GLN	2.8
1	A	105	LYS	2.8
1	A	113	ALA	2.8
1	A	210	THR	2.6
1	A	39	ILE	2.6
1	A	45	ILE	2.6
1	A	274	GLU	2.4
1	A	101	PRO	2.4
1	A	256	ASP	2.4
1	A	271	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	2.3
1	A	414	GLY	2.3
1	A	40	GLY	2.2
1	A	97	ARG	2.2
1	A	200	SER	2.1
1	A	120	TRP	2.1
1	A	46	ASP	2.0
1	A	449	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

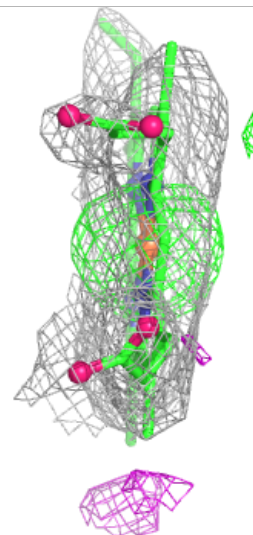
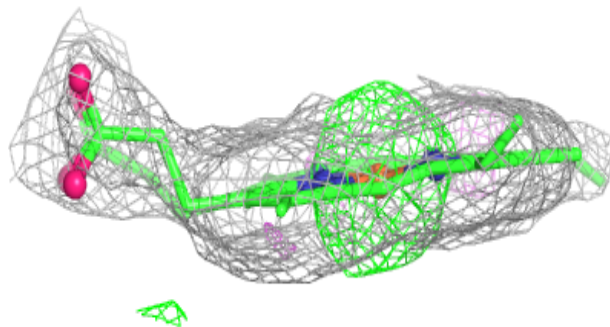
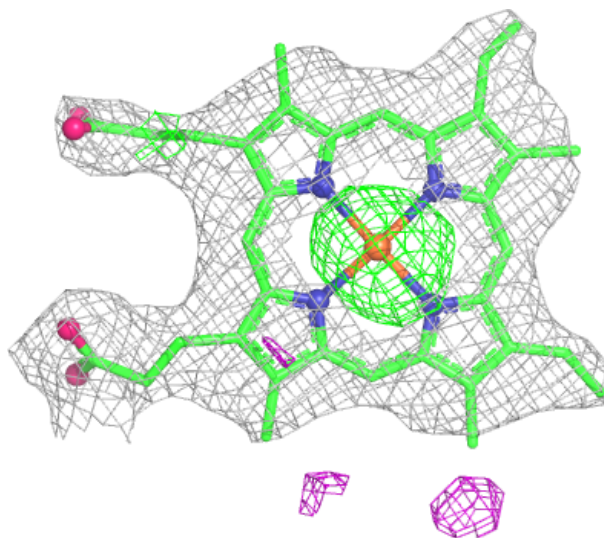
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	505	5/5	0.71	0.13	94,99,99,100	0
3	SO4	A	504	5/5	0.88	0.17	83,83,87,87	0
4	HEM	A	501	43/43	0.95	0.12	26,35,66,80	0
3	SO4	A	503	5/5	0.96	0.08	54,55,59,60	0
2	SM	A	502	1/1	1.00	0.09	31,31,31,31	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 HEM A 501:

$2mF_o-DF_c$ (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.