



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 1, 2018 – 05:13 PM EST

PDB ID : 5VEU
Title : Human Cytochrome P450 3A5 (CYP3A5)
Authors : Hsu, M.-H.; Johnson, E.F.
Deposited on : 2017-04-05
Resolution : 2.91 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

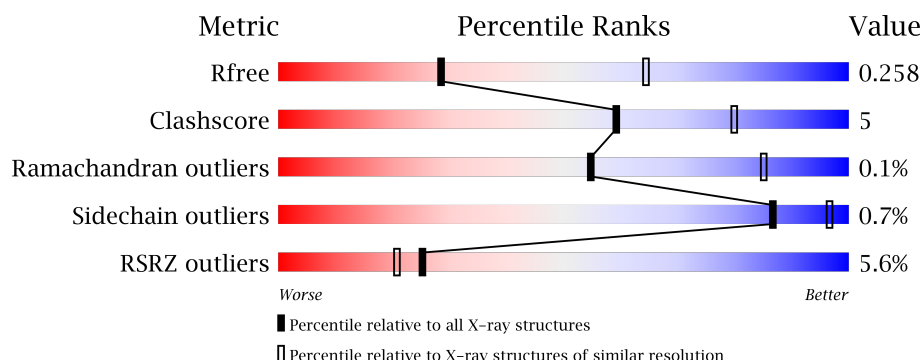
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	480	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>
1	B	480	<div> <div>4%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>
1	C	480	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	D	480	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>•</div> </div>
1	E	480	<div> <div>14%</div> <div>78%</div> <div>14%</div> <div>• 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	480	
1	G	480	
1	H	480	
1	I	480	
1	J	480	
1	K	480	
1	L	480	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RIT	A	602	-	-	-	X
3	RIT	B	602	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 44740 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 3A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3714	2413	616	668	17			
1	B	458	Total	C	N	O	S	0	0	0
			3679	2391	609	662	17			
1	C	469	Total	C	N	O	S	0	0	0
			3773	2448	627	681	17			
1	D	459	Total	C	N	O	S	0	0	0
			3687	2395	610	665	17			
1	E	441	Total	C	N	O	S	0	0	0
			3540	2310	577	636	17			
1	F	456	Total	C	N	O	S	0	0	0
			3661	2381	604	659	17			
1	G	455	Total	C	N	O	S	0	0	0
			3651	2374	602	658	17			
1	H	459	Total	C	N	O	S	0	0	0
			3687	2395	610	665	17			
1	I	464	Total	C	N	O	S	0	0	0
			3732	2423	619	673	17			
1	J	458	Total	C	N	O	S	0	0	0
			3679	2391	609	662	17			
1	K	458	Total	C	N	O	S	0	0	0
			3681	2392	609	663	17			
1	L	448	Total	C	N	O	S	0	0	0
			3590	2339	588	646	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P20815
A	23	ALA	-	expression tag	UNP P20815
A	498	HIS	-	expression tag	UNP P20815
A	499	HIS	-	expression tag	UNP P20815
A	500	HIS	-	expression tag	UNP P20815

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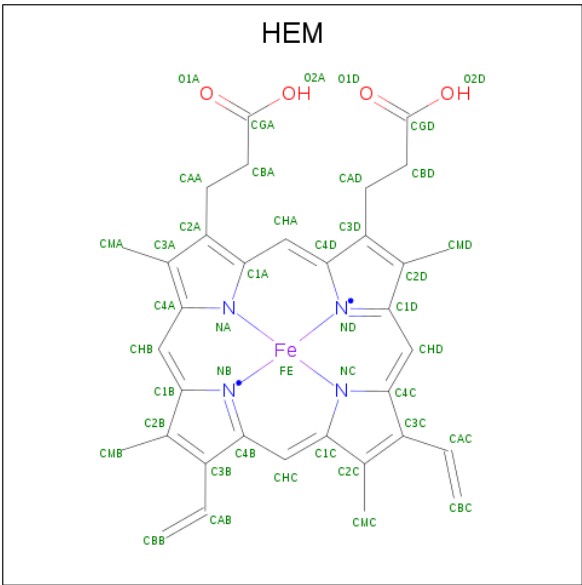
Chain	Residue	Modelled	Actual	Comment	Reference
A	501	HIS	-	expression tag	UNP P20815
B	22	MET	-	initiating methionine	UNP P20815
B	23	ALA	-	expression tag	UNP P20815
B	498	HIS	-	expression tag	UNP P20815
B	499	HIS	-	expression tag	UNP P20815
B	500	HIS	-	expression tag	UNP P20815
B	501	HIS	-	expression tag	UNP P20815
C	22	MET	-	initiating methionine	UNP P20815
C	23	ALA	-	expression tag	UNP P20815
C	498	HIS	-	expression tag	UNP P20815
C	499	HIS	-	expression tag	UNP P20815
C	500	HIS	-	expression tag	UNP P20815
C	501	HIS	-	expression tag	UNP P20815
D	22	MET	-	initiating methionine	UNP P20815
D	23	ALA	-	expression tag	UNP P20815
D	498	HIS	-	expression tag	UNP P20815
D	499	HIS	-	expression tag	UNP P20815
D	500	HIS	-	expression tag	UNP P20815
D	501	HIS	-	expression tag	UNP P20815
E	22	MET	-	initiating methionine	UNP P20815
E	23	ALA	-	expression tag	UNP P20815
E	498	HIS	-	expression tag	UNP P20815
E	499	HIS	-	expression tag	UNP P20815
E	500	HIS	-	expression tag	UNP P20815
E	501	HIS	-	expression tag	UNP P20815
F	22	MET	-	initiating methionine	UNP P20815
F	23	ALA	-	expression tag	UNP P20815
F	498	HIS	-	expression tag	UNP P20815
F	499	HIS	-	expression tag	UNP P20815
F	500	HIS	-	expression tag	UNP P20815
F	501	HIS	-	expression tag	UNP P20815
G	22	MET	-	initiating methionine	UNP P20815
G	23	ALA	-	expression tag	UNP P20815
G	498	HIS	-	expression tag	UNP P20815
G	499	HIS	-	expression tag	UNP P20815
G	500	HIS	-	expression tag	UNP P20815
G	501	HIS	-	expression tag	UNP P20815
H	22	MET	-	initiating methionine	UNP P20815
H	23	ALA	-	expression tag	UNP P20815
H	498	HIS	-	expression tag	UNP P20815
H	499	HIS	-	expression tag	UNP P20815
H	500	HIS	-	expression tag	UNP P20815

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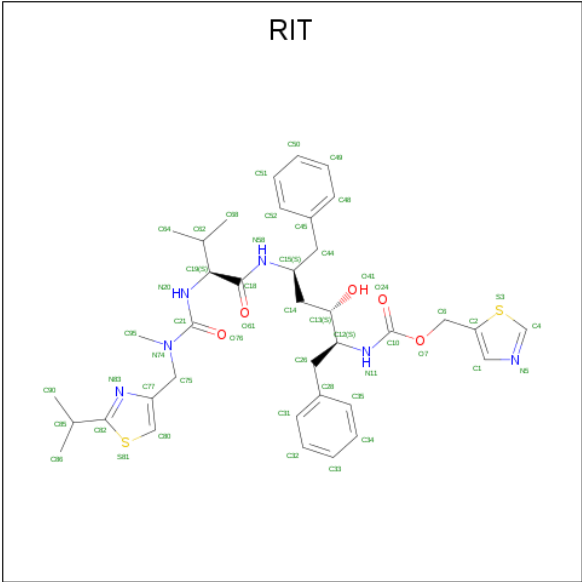
Chain	Residue	Modelled	Actual	Comment	Reference
H	501	HIS	-	expression tag	UNP P20815
I	22	MET	-	initiating methionine	UNP P20815
I	23	ALA	-	expression tag	UNP P20815
I	498	HIS	-	expression tag	UNP P20815
I	499	HIS	-	expression tag	UNP P20815
I	500	HIS	-	expression tag	UNP P20815
I	501	HIS	-	expression tag	UNP P20815
J	22	MET	-	initiating methionine	UNP P20815
J	23	ALA	-	expression tag	UNP P20815
J	498	HIS	-	expression tag	UNP P20815
J	499	HIS	-	expression tag	UNP P20815
J	500	HIS	-	expression tag	UNP P20815
J	501	HIS	-	expression tag	UNP P20815
K	22	MET	-	initiating methionine	UNP P20815
K	23	ALA	-	expression tag	UNP P20815
K	498	HIS	-	expression tag	UNP P20815
K	499	HIS	-	expression tag	UNP P20815
K	500	HIS	-	expression tag	UNP P20815
K	501	HIS	-	expression tag	UNP P20815
L	22	MET	-	initiating methionine	UNP P20815
L	23	ALA	-	expression tag	UNP P20815
L	498	HIS	-	expression tag	UNP P20815
L	499	HIS	-	expression tag	UNP P20815
L	500	HIS	-	expression tag	UNP P20815
L	501	HIS	-	expression tag	UNP P20815

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is RITONAVIR (three-letter code: RIT) (formula: C₃₇H₄₈N₆O₅S₂).

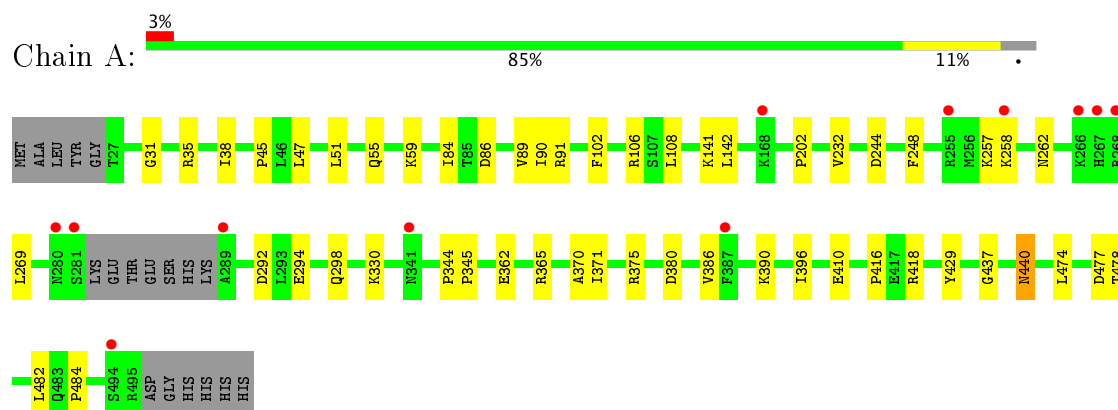


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
3	B	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
3	H	1	Total	C	N	O	S	0	0
			50	37	6	5	2		

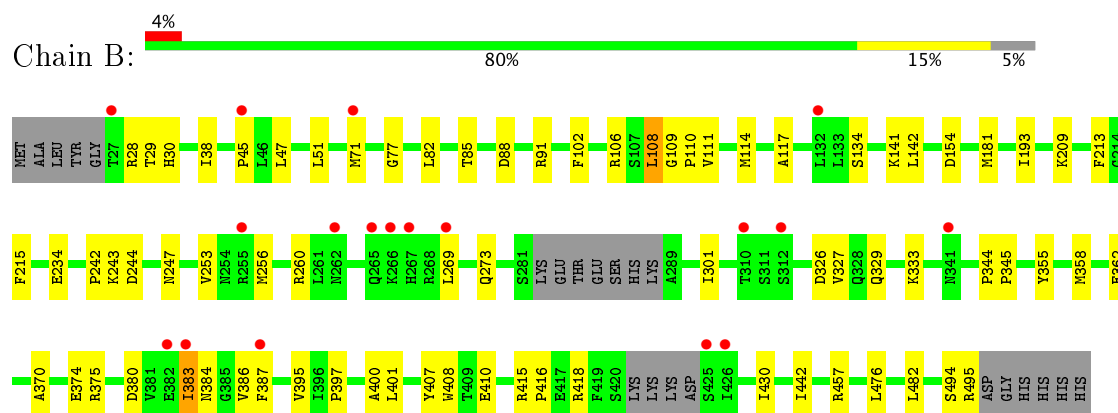
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

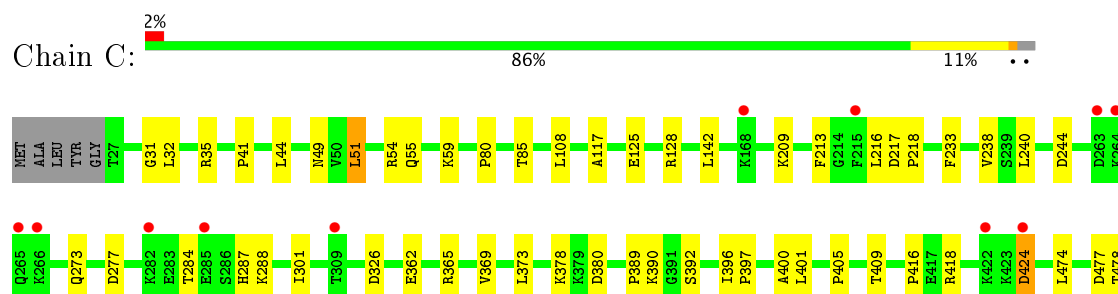
• Molecule 1: Cytochrome P450 3A5

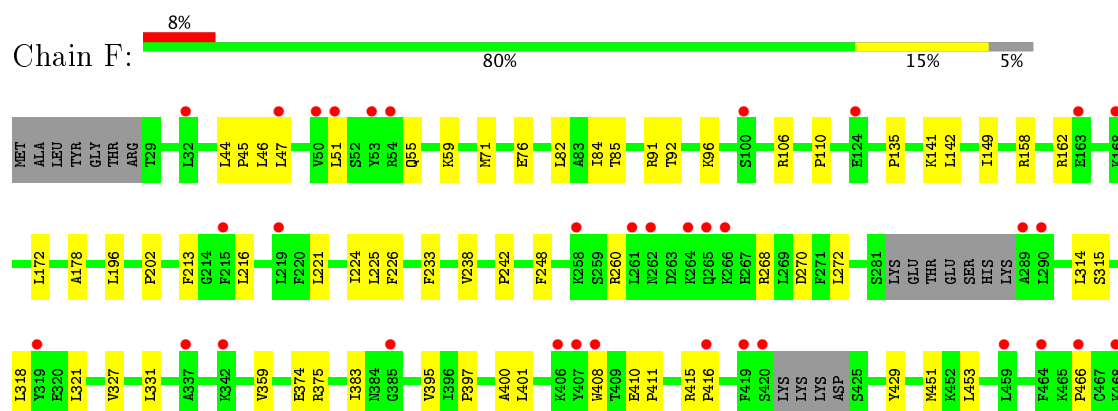


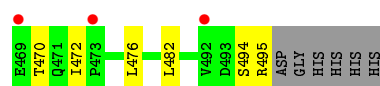
• Molecule 1: Cytochrome P450 3A5



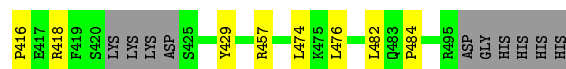
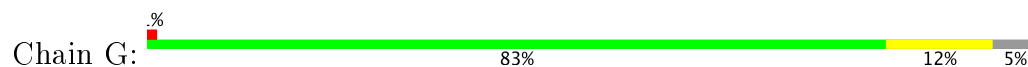
• Molecule 1: Cytochrome P450 3A5



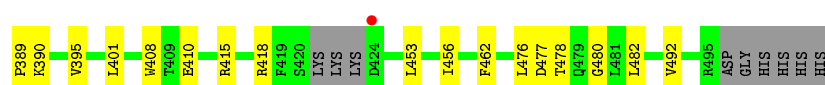
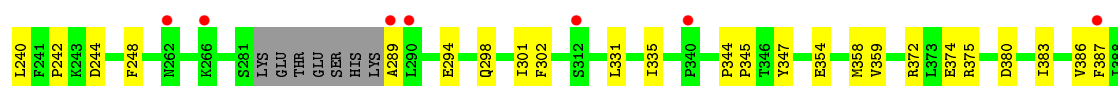
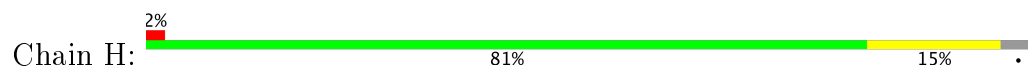




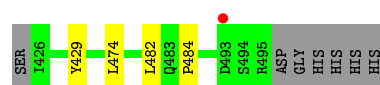
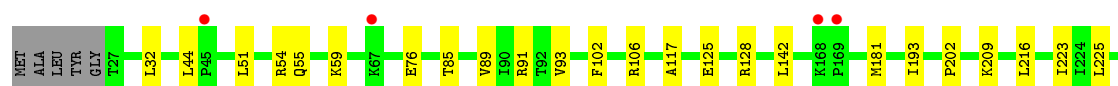
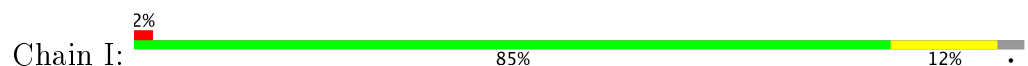
• Molecule 1: Cytochrome P450 3A5



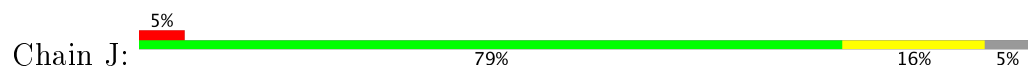
• Molecule 1: Cytochrome P450 3A5

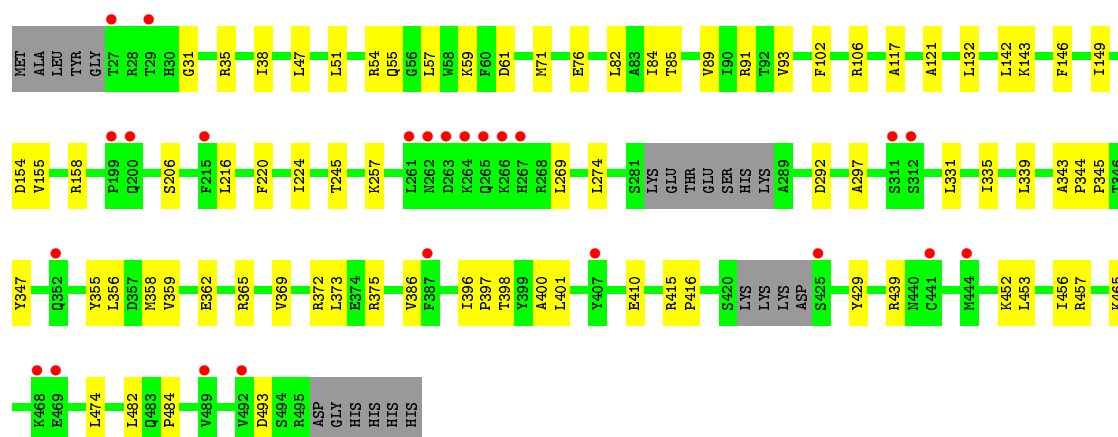


• Molecule 1: Cytochrome P450 3A5

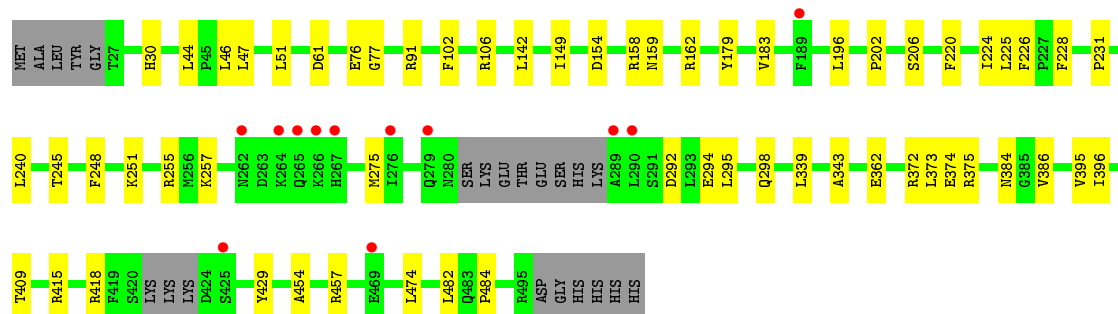
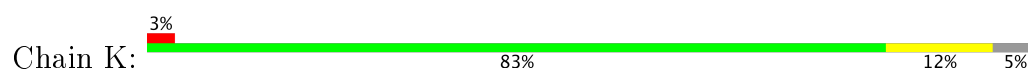


• Molecule 1: Cytochrome P450 3A5

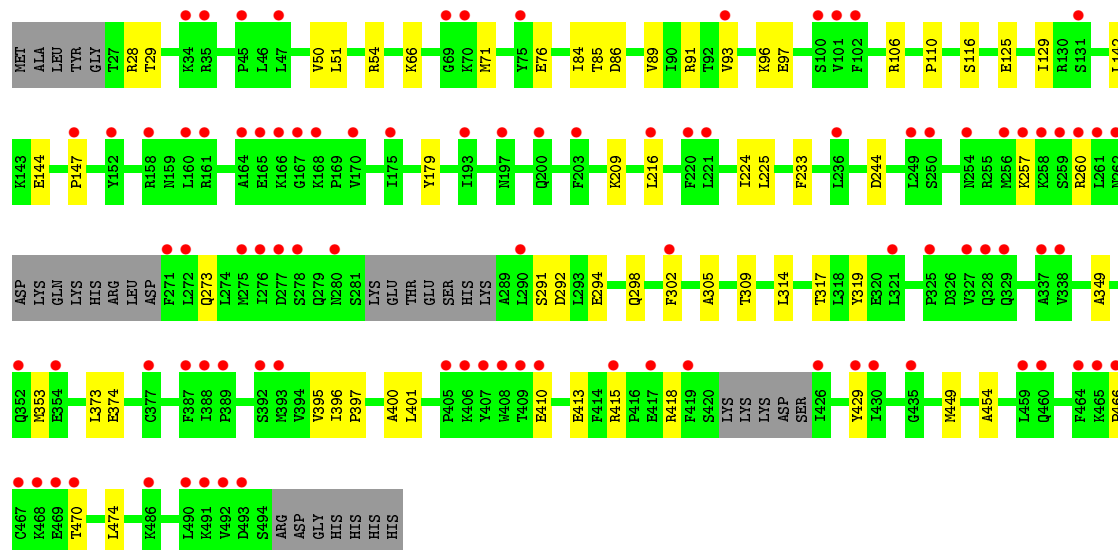
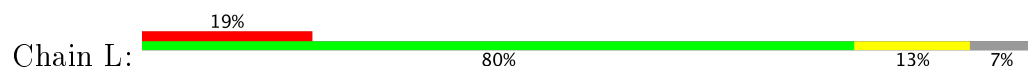




• Molecule 1: Cytochrome P450 3A5



• Molecule 1: Cytochrome P450 3A5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.99Å 198.38Å 234.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.91 39.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.16-2.91) 99.7 (39.16-2.91)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.258 0.214 , 0.258	Depositor DCC
R_{free} test set	7543 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	44740	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: HEM, RIT

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	0.26	0/3803	0.42	0/5148
1	B	0.26	0/3767	0.42	0/5101
1	C	0.26	0/3864	0.43	0/5230
1	D	0.25	0/3775	0.42	0/5112
1	E	0.25	0/3625	0.42	0/4912
1	F	0.25	0/3749	0.41	0/5077
1	G	0.26	0/3737	0.41	0/5060
1	H	0.25	0/3775	0.41	0/5112
1	I	0.26	0/3822	0.42	0/5175
1	J	0.25	0/3767	0.41	0/5101
1	K	0.25	0/3769	0.41	0/5104
1	L	0.24	0/3676	0.41	0/4980
All	All	0.25	0/45129	0.42	0/61112

There are no bond length outliers.

There are no bond angle outliers.

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	3714	0	3810	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3679	0	3766	56	0
1	C	3773	0	3868	33	0
1	D	3687	0	3770	41	0
1	E	3540	0	3618	36	0
1	F	3661	0	3746	42	0
1	G	3651	0	3737	35	0
1	H	3687	0	3770	41	0
1	I	3732	0	3819	34	0
1	J	3679	0	3766	42	0
1	K	3681	0	3765	34	0
1	L	3590	0	3674	36	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0
2	G	43	0	30	2	0
2	H	43	0	30	6	0
2	I	43	0	30	2	0
2	J	43	0	30	2	0
2	K	43	0	30	2	0
2	L	43	0	30	3	0
3	A	50	0	48	5	0
3	B	50	0	48	16	0
3	H	50	0	48	11	0
All	All	44740	0	45613	485	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 5.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:NH1	3:B:602:RIT:H683	1.96	0.81
3:H:602:RIT:H141	3:H:602:RIT:H48	1.61	0.81
1:B:106:ARG:NH1	3:B:602:RIT:C68	2.46	0.79
1:A:38:ILE:HD11	1:A:386:VAL:HG21	1.64	0.79
1:B:117:ALA:HB1	1:B:301:ILE:HG13	1.67	0.76
1:D:410:GLU:OE1	1:D:415:ARG:NH2	2.19	0.76
1:H:408:TRP:HE3	1:H:418:ARG:HD3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ILE:HD11	1:E:386:VAL:HG11	1.69	0.75
1:B:45:PRO:HG2	1:L:216:LEU:HB3	1.66	0.75
1:H:301:ILE:HD13	3:H:602:RIT:H34	1.68	0.75
1:J:369:VAL:HA	1:J:482:LEU:HB2	1.69	0.75
1:B:88:ASP:OD1	1:B:91:ARG:NH1	2.20	0.74
1:F:213:PHE:HE2	1:F:242:PRO:HG3	1.52	0.74
1:G:413:GLU:OE1	1:G:415:ARG:NH2	2.23	0.72
1:C:54:ARG:HD2	1:C:216:LEU:HD11	1.70	0.71
1:L:28:ARG:HG3	1:L:29:THR:HG23	1.73	0.71
1:B:374:GLU:HG2	1:B:395:VAL:HG22	1.72	0.71
1:I:474:LEU:HD11	1:I:484:PRO:HB3	1.72	0.71
1:K:47:LEU:HD13	1:K:225:LEU:HD21	1.72	0.71
1:A:55:GLN:HB3	1:A:59:LYS:HD3	1.73	0.70
1:C:474:LEU:HD11	1:C:484:PRO:HB3	1.72	0.69
1:G:209:LYS:NZ	1:G:244:ASP:OD2	2.25	0.69
1:H:28:ARG:HG3	1:H:29:THR:HG23	1.75	0.69
1:F:76:GLU:OE1	1:F:106:ARG:NH2	2.26	0.68
1:B:408:TRP:HE3	1:B:418:ARG:HD3	1.59	0.68
1:E:409:THR:O	1:E:418:ARG:NH2	2.26	0.68
1:B:111:VAL:HG12	1:B:114:MET:HB2	1.76	0.68
1:C:128:ARG:HB3	1:C:288:LYS:HB2	1.77	0.67
1:C:369:VAL:HA	1:C:482:LEU:HB2	1.75	0.67
1:I:128:ARG:HB3	1:I:288:LYS:HB2	1.76	0.67
1:H:301:ILE:CD1	3:H:602:RIT:H34	2.25	0.67
1:D:142:LEU:HA	1:D:145:MET:HE2	1.78	0.66
1:C:373:LEU:HB2	1:C:396:ILE:HB	1.77	0.66
1:I:32:LEU:HD21	1:I:389:PRO:HG3	1.79	0.65
1:I:260:ARG:HH21	1:I:266:LYS:HE2	1.61	0.65
1:B:410:GLU:OE1	1:B:415:ARG:NH2	2.25	0.64
1:H:374:GLU:HG2	1:H:395:VAL:HG12	1.80	0.64
1:A:474:LEU:HD11	1:A:484:PRO:HB3	1.80	0.64
3:H:602:RIT:C48	3:H:602:RIT:H141	2.27	0.64
1:B:85:THR:HB	1:B:401:LEU:HD21	1.79	0.64
1:H:209:LYS:NZ	1:H:244:ASP:OD2	2.28	0.63
1:L:76:GLU:OE1	1:L:106:ARG:NH2	2.31	0.63
1:I:413:GLU:OE1	1:I:415:ARG:NH2	2.32	0.63
1:E:474:LEU:HD11	1:E:484:PRO:HB3	1.81	0.62
1:C:209:LYS:NZ	1:C:244:ASP:OD2	2.31	0.62
1:J:84:ILE:HD12	1:J:89:VAL:HG12	1.81	0.62
1:F:260:ARG:HE	1:F:272:LEU:HD23	1.64	0.62
1:B:301:ILE:CD1	3:B:602:RIT:H35	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:VAL:HG13	1:J:158:ARG:HH21	1.64	0.62
1:H:408:TRP:CE3	1:H:418:ARG:HD3	2.35	0.61
1:G:474:LEU:HD11	1:G:484:PRO:HB3	1.82	0.61
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.83	0.61
1:D:474:LEU:HD11	1:D:484:PRO:HB3	1.83	0.61
1:F:397:PRO:HB2	1:F:400:ALA:HB3	1.83	0.61
1:C:44:LEU:HD12	1:C:51:LEU:HD23	1.81	0.61
1:I:362:GLU:HG3	1:I:416:PRO:HA	1.83	0.61
1:B:209:LYS:NZ	1:B:244:ASP:OD2	2.34	0.61
1:L:410:GLU:OE1	1:L:415:ARG:NH2	2.32	0.61
1:G:476:LEU:HD23	1:G:482:LEU:HD11	1.83	0.60
2:I:601:HEM:HMC2	2:I:601:HEM:HBC2	1.83	0.60
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.83	0.60
1:E:105:ARG:HH11	2:E:601:HEM:HAA1	1.67	0.60
1:L:413:GLU:O	1:L:418:ARG:NH2	2.35	0.60
1:B:28:ARG:HG3	1:B:29:THR:HG23	1.84	0.60
1:C:32:LEU:HD21	1:C:389:PRO:HG3	1.82	0.60
1:F:375:ARG:NH2	2:F:601:HEM:O1A	2.27	0.60
1:G:55:GLN:HB3	1:G:59:LYS:HD3	1.84	0.60
1:K:474:LEU:HD11	1:K:484:PRO:HB3	1.83	0.60
1:B:106:ARG:NH1	3:B:602:RIT:H681	2.16	0.60
2:J:601:HEM:HBC2	2:J:601:HEM:HMC2	1.83	0.60
1:D:47:LEU:HG	1:D:51:LEU:HD23	1.84	0.59
1:E:279:GLN:NE2	1:E:290:LEU:O	2.35	0.59
1:K:362:GLU:OE2	1:K:418:ARG:NH1	2.32	0.59
1:A:362:GLU:HG3	1:A:416:PRO:HA	1.84	0.59
3:B:602:RIT:H141	3:B:602:RIT:C48	2.31	0.59
1:J:362:GLU:HG3	1:J:416:PRO:HA	1.85	0.59
2:L:601:HEM:HMC2	2:L:601:HEM:HBC2	1.85	0.59
1:B:383:ILE:HG22	1:B:384:ASN:H	1.68	0.59
1:D:55:GLN:HB3	1:D:59:LYS:HD3	1.85	0.59
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.85	0.59
2:K:601:HEM:HMC2	2:K:601:HEM:HBC2	1.83	0.59
1:F:45:PRO:HG2	1:H:216:LEU:HB3	1.85	0.58
1:H:410:GLU:OE1	1:H:415:ARG:NH2	2.36	0.58
2:E:601:HEM:HBC2	2:E:601:HEM:HMC2	1.86	0.58
1:J:71:MET:HE3	1:J:82:LEU:HD11	1.85	0.58
1:J:85:THR:HB	1:J:401:LEU:HD21	1.85	0.58
1:G:154:ASP:OD1	1:G:457:ARG:NH1	2.37	0.58
1:H:375:ARG:NH2	2:H:601:HEM:O1A	2.30	0.58
3:A:602:RIT:H141	3:A:602:RIT:H48	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:HG22	1:D:114:MET:HB2	1.86	0.58
1:D:213:PHE:HE2	1:D:242:PRO:HG3	1.68	0.58
1:E:302:PHE:CD2	2:E:601:HEM:HBC1	2.39	0.58
1:C:362:GLU:HG3	1:C:416:PRO:HA	1.86	0.57
1:A:386:VAL:HG12	1:G:405:PRO:HG2	1.85	0.57
1:J:362:GLU:OE2	1:J:365:ARG:NE	2.27	0.57
1:B:215:PHE:HE2	3:B:602:RIT:H752	1.69	0.57
1:B:355:TYR:HD2	1:B:358:MET:HE3	1.70	0.57
2:F:601:HEM:HBC2	2:F:601:HEM:HMC2	1.85	0.57
1:H:47:LEU:HG	1:H:225:LEU:HD21	1.85	0.57
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.87	0.57
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.86	0.57
2:G:601:HEM:HMC2	2:G:601:HEM:HBC2	1.87	0.57
3:A:602:RIT:C48	3:A:602:RIT:H141	2.35	0.57
1:B:213:PHE:HE2	1:B:242:PRO:HG3	1.69	0.57
1:B:494:SER:OG	1:B:495:ARG:NH1	2.37	0.57
1:J:474:LEU:HD11	1:J:484:PRO:HB3	1.86	0.57
2:K:601:HEM:HMB2	2:K:601:HEM:HBB2	1.87	0.56
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.87	0.56
1:F:466:PRO:HB3	1:F:470:THR:HG21	1.87	0.56
1:L:374:GLU:HG2	1:L:395:VAL:HG22	1.88	0.56
1:A:90:ILE:HG23	1:A:396:ILE:HG12	1.87	0.56
2:D:601:HEM:HBB2	2:D:601:HEM:HMB1	1.86	0.56
2:G:601:HEM:HMB2	2:G:601:HEM:HBB2	1.86	0.56
1:G:71:MET:HE3	1:G:82:LEU:HD11	1.88	0.56
1:D:375:ARG:NH2	2:D:601:HEM:O1A	2.28	0.56
1:F:410:GLU:OE1	1:F:415:ARG:NH2	2.38	0.56
2:J:601:HEM:HBB2	2:J:601:HEM:HMB2	1.86	0.56
1:F:85:THR:HB	1:F:401:LEU:HD21	1.88	0.56
2:I:601:HEM:HMB2	2:I:601:HEM:HBB2	1.87	0.56
1:J:47:LEU:HD13	1:K:47:LEU:HD21	1.87	0.56
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.86	0.55
1:E:157:VAL:HG21	1:E:461:ASN:HD22	1.71	0.55
1:B:38:ILE:HD11	1:B:386:VAL:HG21	1.87	0.55
1:I:262:ASN:HD21	1:I:266:LYS:HD2	1.71	0.55
1:H:128:ARG:NH1	1:H:289:ALA:O	2.39	0.55
2:L:601:HEM:HBB2	2:L:601:HEM:HMB2	1.89	0.55
2:H:601:HEM:HBB2	2:H:601:HEM:HMB2	1.89	0.55
1:G:47:LEU:HD22	1:G:51:LEU:HD21	1.89	0.55
2:F:601:HEM:HBB2	2:F:601:HEM:HMB2	1.88	0.55
2:H:601:HEM:CHA	3:H:602:RIT:H50	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TRP:CE3	1:B:418:ARG:HD3	2.42	0.54
1:E:339:LEU:HB3	1:E:343:ALA:HB3	1.88	0.54
1:K:154:ASP:OD1	1:K:457:ARG:NH1	2.41	0.54
1:G:189:PHE:HD1	1:G:272:LEU:HB2	1.72	0.54
1:F:44:LEU:HD12	1:F:51:LEU:HD23	1.89	0.54
1:H:480:GLY:HA2	3:H:602:RIT:H953	1.90	0.54
3:B:602:RIT:C77	3:B:602:RIT:H20	2.20	0.54
1:I:76:GLU:OE2	1:I:106:ARG:NH2	2.41	0.54
2:E:601:HEM:HMB2	2:E:601:HEM:HBB2	1.90	0.54
1:D:339:LEU:HB3	1:D:343:ALA:HB3	1.89	0.53
1:B:370:ALA:HB2	3:B:602:RIT:H51	1.91	0.53
1:J:339:LEU:HB3	1:J:343:ALA:HB3	1.89	0.53
1:D:362:GLU:OE2	1:D:365:ARG:NE	2.35	0.53
1:G:79:LEU:HD12	1:G:80:PRO:HD2	1.91	0.53
1:B:71:MET:HG2	1:B:82:LEU:HD11	1.91	0.52
1:B:108:LEU:H	1:B:108:LEU:HD13	1.74	0.52
1:A:45:PRO:HG2	1:I:216:LEU:HB3	1.91	0.52
1:J:154:ASP:OD1	1:J:457:ARG:NH1	2.37	0.52
1:K:409:THR:O	1:K:418:ARG:NH2	2.41	0.52
1:L:209:LYS:NZ	1:L:244:ASP:OD2	2.37	0.52
1:C:273:GLN:NE2	1:C:277:ASP:OD1	2.40	0.52
1:J:355:TYR:HD2	1:J:358:MET:HE3	1.75	0.52
1:K:61:ASP:OD1	1:K:372:ARG:NH2	2.43	0.52
1:C:380:ASP:OD1	1:C:390:LYS:N	2.42	0.52
1:H:331:LEU:HD22	1:H:359:VAL:HG21	1.93	0.51
1:J:331:LEU:HD22	1:J:359:VAL:HG21	1.92	0.51
1:C:213:PHE:HE1	1:C:240:LEU:HD12	1.75	0.51
1:A:47:LEU:HD11	1:I:225:LEU:HD11	1.92	0.51
1:A:380:ASP:OD1	1:A:390:LYS:N	2.42	0.51
1:C:397:PRO:HB2	1:C:400:ALA:HB3	1.92	0.51
1:B:253:VAL:HA	1:B:256:MET:HE2	1.92	0.51
1:A:330:LYS:NZ	1:C:405:PRO:O	2.31	0.51
1:F:233:PHE:HB3	1:F:238:VAL:HB	1.91	0.51
1:F:408:TRP:HB2	1:F:411:PRO:HB3	1.91	0.51
1:D:467:CYS:HB3	1:D:491:LYS:HG3	1.92	0.51
1:J:38:ILE:HD11	1:J:386:VAL:HG11	1.93	0.51
1:J:55:GLN:HB3	1:J:59:LYS:HD3	1.92	0.51
1:I:209:LYS:NZ	1:I:244:ASP:OD2	2.32	0.51
1:E:101:VAL:HG12	1:E:379:LYS:HG2	1.93	0.51
1:D:362:GLU:HG3	1:D:416:PRO:HA	1.93	0.51
1:H:380:ASP:OD1	1:H:390:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:257:LYS:NZ	1:L:292:ASP:OD1	2.44	0.51
1:D:369:VAL:HA	1:D:482:LEU:HB2	1.92	0.51
1:G:362:GLU:HG3	1:G:416:PRO:HA	1.93	0.51
1:L:50:VAL:HG21	1:L:224:ILE:HD13	1.93	0.51
1:F:331:LEU:HD22	1:F:359:VAL:HG21	1.94	0.50
1:B:47:LEU:HD21	1:L:225:LEU:HD11	1.92	0.50
1:D:116:SER:O	1:D:298:GLN:NE2	2.41	0.50
1:L:466:PRO:HB3	1:L:470:THR:HG21	1.93	0.50
1:J:220:PHE:CE2	1:J:224:ILE:HD11	2.47	0.50
1:G:61:ASP:OD1	1:G:372:ARG:NH2	2.43	0.50
1:G:415:ARG:O	1:G:418:ARG:HG2	2.11	0.50
1:H:32:LEU:HD11	1:H:389:PRO:HG3	1.94	0.50
1:L:86:ASP:HB3	1:L:89:VAL:HB	1.94	0.50
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.93	0.50
1:F:327:VAL:HG11	1:F:416:PRO:HG2	1.93	0.50
1:F:91:ARG:HG3	1:F:429:TYR:CZ	2.47	0.50
1:I:397:PRO:HB2	1:I:400:ALA:HB3	1.94	0.50
1:J:61:ASP:OD1	1:J:372:ARG:NH2	2.44	0.50
1:B:301:ILE:CD1	3:B:602:RIT:C35	2.90	0.49
1:C:51:LEU:O	1:C:54:ARG:HG3	2.13	0.49
1:K:384:ASN:H	1:K:386:VAL:HG22	1.77	0.49
1:L:125:GLU:O	1:L:129:ILE:HG12	2.12	0.49
1:D:149:ILE:HD13	1:D:450:ASN:HB3	1.94	0.49
1:L:291:SER:H	1:L:294:GLU:HB2	1.77	0.49
1:A:141:LYS:NZ	1:A:269:LEU:HG	2.27	0.49
1:G:213:PHE:HE2	1:G:242:PRO:HG3	1.77	0.49
1:G:373:LEU:HB2	1:G:396:ILE:HB	1.94	0.49
1:F:55:GLN:HB3	1:F:59:LYS:HD3	1.94	0.49
1:K:339:LEU:HB3	1:K:343:ALA:HB3	1.93	0.49
1:L:302:PHE:CD2	2:L:601:HEM:HBC1	2.47	0.49
3:B:602:RIT:N11	3:B:602:RIT:H48	2.27	0.49
1:F:149:ILE:HG22	1:F:453:LEU:HD22	1.95	0.49
1:G:102:PHE:HB3	1:G:375:ARG:HB3	1.93	0.49
1:C:41:PRO:HB2	1:C:49:ASN:ND2	2.28	0.49
1:J:143:LYS:HG2	1:J:347:TYR:CG	2.48	0.48
1:A:294:GLU:O	1:A:298:GLN:HG2	2.14	0.48
1:I:91:ARG:HG3	1:I:429:TYR:CZ	2.49	0.48
1:B:215:PHE:CE2	3:B:602:RIT:H752	2.48	0.48
1:D:409:THR:O	1:D:418:ARG:NH2	2.47	0.48
1:H:354:GLU:O	1:H:358:MET:HG3	2.13	0.48
1:L:260:ARG:HH12	1:L:273:GLN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:HG3	1:B:416:PRO:HA	1.94	0.48
1:C:80:PRO:HG2	1:C:392:SER:HB3	1.95	0.48
1:D:359:VAL:HG13	1:D:414:PHE:HZ	1.78	0.48
1:H:61:ASP:OD2	1:H:372:ARG:HD3	2.14	0.48
1:J:149:ILE:HG22	1:J:453:LEU:HD22	1.96	0.48
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.95	0.48
1:D:357:ASP:O	1:D:361:ASN:ND2	2.46	0.48
1:K:158:ARG:HE	1:K:162:ARG:HH21	1.60	0.48
1:D:397:PRO:HB2	1:D:400:ALA:HB3	1.96	0.48
1:F:158:ARG:HH21	1:F:162:ARG:HH22	1.61	0.48
1:H:150:ALA:HA	1:H:453:LEU:HD21	1.96	0.48
1:B:141:LYS:NZ	1:B:269:LEU:HG	2.29	0.48
1:E:377:CYS:SG	1:E:388:ILE:HD11	2.54	0.48
1:K:206:SER:HB3	1:K:245:THR:HG23	1.96	0.48
1:G:91:ARG:HG3	1:G:429:TYR:CZ	2.49	0.48
1:B:109:GLY:O	1:B:111:VAL:HG23	2.13	0.48
1:E:133:LEU:HD22	1:E:271:PHE:HE1	1.78	0.48
1:F:268:ARG:HH11	1:F:270:ASP:HB3	1.78	0.48
1:J:91:ARG:HG3	1:J:429:TYR:OH	2.13	0.48
1:K:220:PHE:CE2	1:K:224:ILE:HD11	2.48	0.48
1:L:110:PRO:HG3	1:L:233:PHE:HD2	1.78	0.47
1:H:294:GLU:O	1:H:298:GLN:HG2	2.14	0.47
1:K:159:ASN:ND2	1:K:196:LEU:O	2.47	0.47
1:H:202:PRO:HB2	1:H:248:PHE:CZ	2.50	0.47
1:I:362:GLU:OE2	1:I:365:ARG:NE	2.40	0.47
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.95	0.47
1:J:102:PHE:HB3	1:J:375:ARG:HB3	1.96	0.47
1:B:30:HIS:NE2	1:B:77:GLY:O	2.42	0.47
1:C:117:ALA:HB1	1:C:301:ILE:HG13	1.97	0.47
1:J:257:LYS:NZ	1:J:292:ASP:OD1	2.48	0.47
1:H:160:LEU:HD13	1:H:175:ILE:HD13	1.96	0.47
1:K:91:ARG:HG3	1:K:429:TYR:CZ	2.50	0.47
1:L:51:LEU:O	1:L:54:ARG:HG2	2.14	0.47
1:C:362:GLU:OE2	1:C:365:ARG:NE	2.45	0.47
1:C:85:THR:HB	1:C:401:LEU:HD21	1.97	0.47
1:I:260:ARG:HD3	1:I:273:GLN:OE1	2.15	0.47
1:J:31:GLY:O	1:J:35:ARG:HG2	2.15	0.47
1:D:477:ASP:OD1	1:D:478:THR:N	2.48	0.47
2:H:601:HEM:C1D	3:H:602:RIT:H1	2.49	0.47
1:J:410:GLU:OE1	1:J:415:ARG:NH2	2.48	0.47
1:L:373:LEU:HB2	1:L:396:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HB3	1:G:45:PRO:HG2	1.97	0.46
1:D:108:LEU:HD12	1:D:109:GLY:H	1.80	0.46
1:D:110:PRO:HA	1:D:234:GLU:OE1	2.16	0.46
1:E:110:PRO:HD3	1:E:230:THR:HG23	1.97	0.46
1:L:96:LYS:HG2	1:L:97:GLU:HG3	1.97	0.46
1:E:356:LEU:HD21	1:E:452:LYS:HB3	1.96	0.46
1:L:319:TYR:CZ	1:L:474:LEU:HB2	2.50	0.46
1:L:84:ILE:HD12	1:L:89:VAL:HG12	1.97	0.46
1:B:329:GLN:HG2	1:B:333:LYS:HE3	1.97	0.46
2:B:601:HEM:CAA	3:B:602:RIT:H50	2.46	0.46
3:H:602:RIT:O61	3:H:602:RIT:H441	2.14	0.46
1:I:223:ILE:HD11	1:I:233:PHE:HD2	1.80	0.46
1:C:409:THR:O	1:C:418:ARG:NH1	2.48	0.46
1:D:128:ARG:HH21	1:D:289:ALA:N	2.12	0.46
1:I:202:PRO:HB2	1:I:248:PHE:CZ	2.50	0.46
1:K:257:LYS:NZ	1:K:292:ASP:OD1	2.49	0.46
1:H:38:ILE:HD11	1:H:386:VAL:HG21	1.98	0.46
1:H:214:GLY:HA2	3:H:602:RIT:C95	2.45	0.46
1:A:477:ASP:OD1	1:A:478:THR:N	2.48	0.46
1:A:370:ALA:HB2	3:A:602:RIT:C51	2.45	0.46
1:A:371:ILE:HG13	1:A:482:LEU:HD21	1.98	0.46
1:F:110:PRO:HG3	1:F:233:PHE:HB2	1.97	0.46
1:F:92:THR:HA	1:F:96:LYS:HB3	1.98	0.46
1:G:142:LEU:HA	1:G:142:LEU:HD13	1.84	0.46
1:C:55:GLN:HB2	1:C:59:LYS:HE3	1.98	0.46
1:E:384:ASN:HB3	1:E:385:GLY:H	1.62	0.46
1:I:51:LEU:O	1:I:54:ARG:HG3	2.15	0.46
1:B:243:LYS:O	1:B:247:ASN:ND2	2.38	0.45
1:A:232:VAL:HG22	1:E:228:PHE:HD1	1.80	0.45
1:H:477:ASP:OD1	1:H:478:THR:N	2.49	0.45
1:B:326:ASP:OD1	1:B:327:VAL:N	2.49	0.45
1:B:301:ILE:HD13	3:B:602:RIT:H34	1.98	0.45
1:C:284:THR:HG23	1:C:287:HIS:H	1.81	0.45
1:D:85:THR:HB	1:D:401:LEU:HD21	1.98	0.45
1:A:31:GLY:O	1:A:35:ARG:HB2	2.16	0.45
1:F:476:LEU:HD23	1:F:482:LEU:HD11	1.98	0.45
1:H:213:PHE:HE2	1:H:242:PRO:HG3	1.81	0.45
1:L:91:ARG:HG3	1:L:429:TYR:OH	2.16	0.45
1:C:477:ASP:OD1	1:C:478:THR:N	2.49	0.45
1:G:279:GLN:HG2	1:G:290:LEU:O	2.17	0.45
1:H:85:THR:HB	1:H:401:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:ALA:HB2	1:J:297:ALA:HB1	1.98	0.45
1:K:102:PHE:HB3	1:K:375:ARG:HB3	1.98	0.45
1:K:415:ARG:O	1:K:418:ARG:HG2	2.16	0.45
1:E:156:LEU:HD13	1:E:179:TYR:HB2	1.99	0.45
1:D:265:GLN:HG3	1:D:266:LYS:HG3	1.98	0.45
1:J:132:LEU:O	1:J:274:LEU:HD21	2.15	0.45
1:J:373:LEU:HB2	1:J:396:ILE:HB	1.99	0.45
1:J:397:PRO:HB2	1:J:400:ALA:HB3	1.98	0.45
1:A:362:GLU:OE2	1:A:365:ARG:NE	2.30	0.45
1:F:216:LEU:HA	1:F:221:LEU:HD22	1.99	0.45
1:B:181:MET:HG3	1:B:193:ILE:HD11	1.99	0.45
1:B:260:ARG:NH1	1:B:273:GLN:HB2	2.32	0.45
1:I:89:VAL:HG22	1:I:384:ASN:HB2	1.99	0.45
1:K:294:GLU:O	1:K:298:GLN:HG2	2.16	0.45
1:L:349:ALA:O	1:L:353:MET:HG3	2.17	0.45
1:E:158:ARG:HG2	1:E:162:ARG:HH21	1.82	0.44
1:E:142:LEU:HD12	1:E:449:MET:SD	2.57	0.44
1:F:318:LEU:HD23	1:F:321:LEU:HD12	1.98	0.44
1:F:494:SER:HB3	1:F:495:ARG:NH1	2.32	0.44
1:I:482:LEU:HD12	1:I:482:LEU:HA	1.86	0.44
1:C:233:PHE:HB3	1:C:238:VAL:HB	1.99	0.44
1:H:71:MET:HE2	1:H:82:LEU:HD11	1.98	0.44
1:I:262:ASN:ND2	1:I:266:LYS:HD2	2.32	0.44
1:L:314:LEU:O	1:L:317:THR:OG1	2.30	0.44
1:B:110:PRO:HA	1:B:234:GLU:OE1	2.17	0.44
1:E:91:ARG:HG3	1:E:429:TYR:OH	2.17	0.44
1:F:221:LEU:O	1:F:225:LEU:HG	2.18	0.44
1:I:44:LEU:HD12	1:I:51:LEU:HD23	2.00	0.44
1:C:326:ASP:OD1	1:C:326:ASP:N	2.49	0.44
1:G:410:GLU:HB3	1:G:413:GLU:HG3	2.00	0.44
1:J:465:LYS:NZ	1:J:493:ASP:OD2	2.45	0.44
1:A:202:PRO:HB2	1:A:248:PHE:CZ	2.53	0.44
1:B:106:ARG:HD3	3:B:602:RIT:H641	2.00	0.44
1:B:380:ASP:HB3	1:B:387:PHE:CZ	2.53	0.44
1:D:220:PHE:CE2	1:D:224:ILE:HD11	2.53	0.44
1:K:179:TYR:CZ	1:K:454:ALA:HB2	2.53	0.44
1:E:93:VAL:HA	1:E:102:PHE:CD2	2.53	0.44
1:H:30:HIS:NE2	1:H:77:GLY:O	2.50	0.44
1:E:71:MET:HG2	1:E:84:ILE:HG22	2.00	0.43
1:G:96:LYS:HG2	1:G:97:GLU:HG3	2.00	0.43
1:A:437:GLY:O	1:A:440:ASN:ND2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:LEU:HD21	1:K:46:LEU:HD23	1.99	0.43
1:D:494:SER:HB3	1:D:495:ARG:NH1	2.33	0.43
1:F:46:LEU:HD11	1:F:226:PHE:HE1	1.84	0.43
1:G:362:GLU:OE2	1:G:418:ARG:HD2	2.18	0.43
1:K:149:ILE:HG12	1:K:183:VAL:HG13	2.00	0.43
1:G:228:PHE:HB2	1:K:231:PRO:HB2	2.00	0.43
1:B:326:ASP:N	1:B:326:ASP:OD1	2.51	0.43
1:C:31:GLY:O	1:C:35:ARG:HG3	2.18	0.43
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.88	0.43
1:E:365:ARG:NH1	1:E:402:HIS:O	2.51	0.43
1:E:397:PRO:HB2	1:E:400:ALA:HB3	1.99	0.43
1:I:389:PRO:HG2	1:I:392:SER:OG	2.19	0.43
1:J:76:GLU:OE1	1:J:106:ARG:NH2	2.51	0.43
1:L:179:TYR:CE2	1:L:454:ALA:HB2	2.53	0.43
1:D:134:SER:HA	1:D:442:ILE:HD11	2.01	0.43
1:E:372:ARG:HD2	1:E:395:VAL:HG13	2.01	0.43
1:F:470:THR:HG22	1:F:472:ILE:HG13	2.01	0.43
1:I:117:ALA:HB1	1:I:301:ILE:HG13	2.01	0.43
1:J:91:ARG:HG3	1:J:429:TYR:CZ	2.54	0.43
1:L:142:LEU:HD12	1:L:449:MET:SD	2.59	0.43
1:C:244:ASP:N	1:C:244:ASP:OD1	2.52	0.43
1:D:99:TYR:HD1	1:D:127:LYS:HE2	1.84	0.43
1:F:71:MET:HB3	1:F:71:MET:HE2	1.85	0.43
1:F:47:LEU:HA	1:F:225:LEU:HD22	1.99	0.43
1:B:355:TYR:CD2	1:B:358:MET:HE3	2.51	0.43
1:D:379:LYS:HA	1:D:390:LYS:HG3	2.00	0.43
1:L:85:THR:HB	1:L:401:LEU:HD21	2.01	0.43
1:L:84:ILE:HD11	1:L:93:VAL:HG21	2.01	0.43
1:J:51:LEU:O	1:J:54:ARG:HG2	2.19	0.43
1:K:226:PHE:HB3	1:K:228:PHE:CZ	2.54	0.43
1:D:92:THR:HG23	1:D:96:LYS:HD3	2.01	0.42
1:E:30:HIS:NE2	1:E:45:PRO:O	2.52	0.42
1:F:314:LEU:HG	1:F:451:MET:HG2	2.00	0.42
1:A:410:GLU:O	1:A:418:ARG:NH2	2.52	0.42
1:E:84:ILE:HD12	1:E:89:VAL:HG12	2.01	0.42
1:I:93:VAL:HG13	1:I:102:PHE:CG	2.54	0.42
1:J:335:ILE:HD13	1:J:456:ILE:HA	2.01	0.42
2:H:601:HEM:CHA	3:H:602:RIT:C50	2.96	0.42
1:J:269:LEU:HA	1:J:269:LEU:HD12	1.84	0.42
1:B:301:ILE:HD12	3:B:602:RIT:H35	2.01	0.42
1:E:375:ARG:NH2	2:E:601:HEM:O1A	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:PHE:CE2	1:H:224:ILE:HD11	2.54	0.42
1:H:302:PHE:CD2	2:H:601:HEM:HBC1	2.55	0.42
1:J:93:VAL:HG13	1:J:102:PHE:CG	2.53	0.42
1:L:116:SER:O	1:L:298:GLN:NE2	2.42	0.42
2:A:601:HEM:C1A	3:A:602:RIT:H50	2.54	0.42
1:B:407:TYR:CE1	1:B:430:ILE:HG13	2.55	0.42
1:G:85:THR:HB	1:G:401:LEU:HD21	2.01	0.42
1:I:125:GLU:OE1	1:I:128:ARG:NH2	2.45	0.42
1:I:373:LEU:HB2	1:I:396:ILE:HB	2.02	0.42
1:I:369:VAL:HA	1:I:482:LEU:HB2	2.00	0.42
1:D:408:TRP:HB2	1:D:411:PRO:HB3	2.01	0.42
1:K:202:PRO:HB2	1:K:248:PHE:CZ	2.54	0.42
1:D:260:ARG:NH1	1:D:267:HIS:HA	2.34	0.42
1:G:326:ASP:OD1	1:G:326:ASP:N	2.53	0.42
1:H:335:ILE:HD13	1:H:456:ILE:HA	2.02	0.42
1:H:143:LYS:HE2	1:H:347:TYR:CE2	2.55	0.42
1:J:121:ALA:O	1:J:439:ARG:NH1	2.44	0.42
1:J:206:SER:HB3	1:J:245:THR:HG23	2.02	0.42
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.90	0.42
1:E:315:SER:HB3	1:E:488:ILE:HD12	2.02	0.42
1:F:172:LEU:HD23	1:F:315:SER:HA	2.01	0.42
1:G:327:VAL:HG13	1:G:355:TYR:OH	2.19	0.42
1:H:102:PHE:HB3	1:H:375:ARG:HB3	2.01	0.42
1:I:327:VAL:HG11	1:I:414:PHE:HE2	1.85	0.42
1:K:220:PHE:HB2	1:K:240:LEU:HD11	2.01	0.42
1:K:373:LEU:HB2	1:K:396:ILE:HB	2.02	0.42
1:A:244:ASP:N	1:A:244:ASP:OD1	2.51	0.42
1:A:258:LYS:O	1:A:262:ASN:ND2	2.50	0.42
1:B:38:ILE:HD11	1:B:386:VAL:HG11	2.01	0.42
1:C:125:GLU:OE2	1:C:288:LYS:NZ	2.43	0.42
1:E:104:ASN:HA	1:E:439:ARG:NH1	2.35	0.42
1:L:260:ARG:NH1	1:L:273:GLN:HB2	2.34	0.42
1:L:397:PRO:HB2	1:L:400:ALA:HB3	2.02	0.42
1:D:125:GLU:O	1:D:129:ILE:HG12	2.19	0.42
1:F:221:LEU:HA	1:F:224:ILE:HD12	2.02	0.42
1:G:108:LEU:HD12	1:G:109:GLY:H	1.85	0.42
1:H:301:ILE:CD1	3:H:602:RIT:C34	2.97	0.42
1:L:71:MET:HE3	1:L:71:MET:HB3	1.92	0.42
1:A:257:LYS:NZ	1:A:292:ASP:OD1	2.53	0.41
1:B:362:GLU:OE2	1:B:418:ARG:NH1	2.52	0.41
1:E:85:THR:HB	1:E:401:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ASP:OD1	1:E:478:THR:N	2.53	0.41
1:F:84:ILE:O	1:F:397:PRO:HD2	2.20	0.41
1:F:82:LEU:HD23	1:F:383:ILE:HD11	2.00	0.41
1:G:344:PRO:HA	1:G:345:PRO:HD3	1.88	0.41
1:G:76:GLU:OE1	1:G:106:ARG:NH2	2.52	0.41
1:H:344:PRO:HA	1:H:345:PRO:HD3	1.88	0.41
1:K:482:LEU:HA	1:K:482:LEU:HD12	1.87	0.41
3:B:602:RIT:H142	3:B:602:RIT:H643	2.02	0.41
1:F:158:ARG:HE	1:F:162:ARG:NH2	2.19	0.41
1:L:144:GLU:O	1:L:147:PRO:HD2	2.20	0.41
1:A:370:ALA:HB2	3:A:602:RIT:H51	2.02	0.41
1:E:105:ARG:HA	1:E:375:ARG:HA	2.01	0.41
1:E:44:LEU:HD22	1:E:51:LEU:HD23	2.03	0.41
1:F:221:LEU:HD21	1:H:46:LEU:HD22	2.01	0.41
1:H:476:LEU:HD23	1:H:482:LEU:HD11	2.02	0.41
1:I:279:GLN:HG2	1:I:290:LEU:O	2.21	0.41
1:B:154:ASP:OD1	1:B:457:ARG:NH1	2.53	0.41
1:C:213:PHE:CE1	1:C:240:LEU:HD12	2.53	0.41
1:H:462:PHE:HB3	1:H:492:VAL:HG23	2.03	0.41
1:K:44:LEU:HD22	1:K:51:LEU:HD23	2.01	0.41
1:L:66:LYS:HE2	1:L:66:LYS:HB3	1.87	0.41
1:D:96:LYS:HG2	1:D:97:GLU:HG3	2.03	0.41
1:E:134:SER:HA	1:E:442:ILE:HD11	2.02	0.41
1:F:482:LEU:HA	1:F:482:LEU:HD12	1.86	0.41
1:I:223:ILE:HD11	1:I:233:PHE:CD2	2.55	0.41
1:K:374:GLU:HG2	1:K:395:VAL:HG22	2.02	0.41
1:F:135:PRO:O	1:F:141:LYS:HD2	2.21	0.41
1:F:374:GLU:HG2	1:F:395:VAL:HG22	2.03	0.41
1:J:57:LEU:HD12	1:J:57:LEU:HA	1.91	0.41
1:K:251:LYS:O	1:K:255:ARG:HG3	2.21	0.41
1:K:46:LEU:HG	1:K:225:LEU:HD22	2.01	0.41
1:K:275:MET:HE3	1:K:295:LEU:HG	2.03	0.41
1:C:378:LYS:O	1:C:390:LYS:HG3	2.21	0.41
1:I:55:GLN:HG3	1:I:59:LYS:HD3	2.03	0.41
1:A:91:ARG:HG3	1:A:429:TYR:CZ	2.55	0.41
1:B:47:LEU:HG	1:B:51:LEU:CD2	2.51	0.41
1:B:482:LEU:HA	1:B:482:LEU:HD12	1.80	0.41
1:D:76:GLU:OE1	1:D:106:ARG:NH2	2.54	0.41
1:J:356:LEU:HD21	1:J:452:LYS:HB3	2.03	0.41
1:F:178:ALA:HB1	1:F:196:LEU:HA	2.03	0.41
1:L:305:ALA:O	1:L:309:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HB3	1:G:46:LEU:HD13	2.03	0.41
1:E:157:VAL:HG23	1:E:462:PHE:CE2	2.56	0.41
1:G:99:TYR:HD1	1:G:127:LYS:HE2	1.86	0.41
1:H:383:ILE:O	1:H:386:VAL:HG22	2.20	0.41
1:I:181:MET:HG3	1:I:193:ILE:HD11	2.03	0.41
1:K:76:GLU:OE1	1:K:106:ARG:NH2	2.54	0.41
1:K:30:HIS:HE1	1:K:77:GLY:O	2.04	0.41
1:D:202:PRO:HB2	1:D:248:PHE:CZ	2.56	0.40
1:G:226:PHE:HB3	1:G:228:PHE:CZ	2.56	0.40
1:I:85:THR:HB	1:I:401:LEU:HD21	2.03	0.40
1:D:213:PHE:CE2	1:D:242:PRO:HG3	2.53	0.40
1:D:183:VAL:HG11	1:D:450:ASN:HD22	1.87	0.40
1:A:84:ILE:HD12	1:A:89:VAL:HG12	2.03	0.40
1:B:134:SER:HA	1:B:442:ILE:HD11	2.04	0.40
1:D:244:ASP:OD1	1:D:244:ASP:N	2.54	0.40
1:H:116:SER:O	1:H:298:GLN:NE2	2.45	0.40
1:A:371:ILE:HG13	1:A:482:LEU:CD2	2.51	0.40
1:B:213:PHE:CE2	1:B:242:PRO:HG3	2.53	0.40
1:E:105:ARG:O	1:E:376:THR:OG1	2.30	0.40
1:F:202:PRO:HB2	1:F:248:PHE:CZ	2.56	0.40
1:J:396:ILE:O	1:J:398:THR:N	2.55	0.40
1:A:86:ASP:O	1:A:90:ILE:HG13	2.21	0.40
1:B:244:ASP:OD1	1:B:244:ASP:N	2.54	0.40
1:B:344:PRO:HA	1:B:345:PRO:HD3	1.88	0.40
1:D:383:ILE:O	1:D:386:VAL:HG22	2.21	0.40
1:G:92:THR:HA	1:G:96:LYS:HB3	2.04	0.40
1:J:344:PRO:HA	1:J:345:PRO:HD3	1.90	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	458/480 (95%)	441 (96%)	17 (4%)	0	100	100
1	B	452/480 (94%)	430 (95%)	21 (5%)	1 (0%)	51	81
1	C	467/480 (97%)	449 (96%)	17 (4%)	1 (0%)	51	81
1	D	453/480 (94%)	432 (95%)	21 (5%)	0	100	100
1	E	431/480 (90%)	412 (96%)	18 (4%)	1 (0%)	51	81
1	F	450/480 (94%)	431 (96%)	19 (4%)	0	100	100
1	G	447/480 (93%)	432 (97%)	15 (3%)	0	100	100
1	H	453/480 (94%)	436 (96%)	17 (4%)	0	100	100
1	I	460/480 (96%)	441 (96%)	19 (4%)	0	100	100
1	J	452/480 (94%)	434 (96%)	18 (4%)	0	100	100
1	K	452/480 (94%)	432 (96%)	20 (4%)	0	100	100
1	L	440/480 (92%)	424 (96%)	16 (4%)	0	100	100
All	All	5415/5760 (94%)	5194 (96%)	218 (4%)	3 (0%)	55	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	424	ASP
1	B	383	ILE
1	E	353	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/434 (96%)	415 (99%)	4 (1%)	80	94
1	B	415/434 (96%)	412 (99%)	3 (1%)	87	96
1	C	426/434 (98%)	420 (99%)	6 (1%)	71	91
1	D	416/434 (96%)	412 (99%)	4 (1%)	80	94
1	E	399/434 (92%)	391 (98%)	8 (2%)	60	86
1	F	413/434 (95%)	412 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	412/434 (95%)	411 (100%)	1 (0%)	94	98
1	H	416/434 (96%)	412 (99%)	4 (1%)	80	94
1	I	421/434 (97%)	419 (100%)	2 (0%)	91	97
1	J	415/434 (96%)	412 (99%)	3 (1%)	87	96
1	K	415/434 (96%)	414 (100%)	1 (0%)	94	98
1	L	405/434 (93%)	405 (100%)	0	100	100
All	All	4972/5208 (96%)	4935 (99%)	37 (1%)	87	96

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	106	ARG
1	A	142	LEU
1	A	440	ASN
1	B	108	LEU
1	B	142	LEU
1	B	476	LEU
1	C	51	LEU
1	C	108	LEU
1	C	142	LEU
1	C	217	ASP
1	C	424	ASP
1	C	482	LEU
1	D	51	LEU
1	D	146	PHE
1	D	372	ARG
1	D	482	LEU
1	E	54	ARG
1	E	57	LEU
1	E	101	VAL
1	E	105	ARG
1	E	108	LEU
1	E	142	LEU
1	E	269	LEU
1	E	476	LEU
1	F	142	LEU
1	G	142	LEU
1	H	51	LEU
1	H	142	LEU

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Mol	Chain	Res	Type
1	H	240	LEU
1	H	387	PHE
1	I	142	LEU
1	I	237	ASN
1	J	142	LEU
1	J	146	PHE
1	J	216	LEU
1	K	142	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	460	GLN
1	H	265	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	A	601	1,3	28,50,50	1.78	4 (14%)	17,82,82	1.51	3 (17%)
3	RIT	A	602	2	48,53,53	0.50	1 (2%)	50,71,71	0.82	2 (4%)
2	HEM	B	601	1,3	28,50,50	1.80	4 (14%)	17,82,82	1.51	4 (23%)
3	RIT	B	602	2	48,53,53	0.50	1 (2%)	50,71,71	0.57	0
2	HEM	C	601	1	28,50,50	1.77	4 (14%)	17,82,82	1.44	1 (5%)
2	HEM	D	601	1	28,50,50	1.79	4 (14%)	17,82,82	1.53	5 (29%)
2	HEM	E	601	1	28,50,50	1.76	4 (14%)	17,82,82	1.54	3 (17%)
2	HEM	F	601	1	28,50,50	1.76	4 (14%)	17,82,82	1.51	4 (23%)
2	HEM	G	601	1	28,50,50	1.77	4 (14%)	17,82,82	1.48	2 (11%)
2	HEM	H	601	1,3	28,50,50	1.83	4 (14%)	17,82,82	1.99	6 (35%)
3	RIT	H	602	2	48,53,53	0.54	1 (2%)	50,71,71	0.98	3 (6%)
2	HEM	I	601	1	28,50,50	1.77	4 (14%)	17,82,82	1.46	2 (11%)
2	HEM	J	601	1	28,50,50	1.76	4 (14%)	17,82,82	1.51	2 (11%)
2	HEM	K	601	1	28,50,50	1.75	4 (14%)	17,82,82	1.54	3 (17%)
2	HEM	L	601	1	28,50,50	1.75	4 (14%)	17,82,82	1.53	2 (11%)

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	A	601	1,3	-	0/6/54/54	0/0/8/8
3	RIT	A	602	2	-	0/49/53/53	0/4/4/4
2	HEM	B	601	1,3	-	0/6/54/54	0/0/8/8
3	RIT	B	602	2	-	0/49/53/53	0/4/4/4
2	HEM	C	601	1	-	0/6/54/54	0/0/8/8
2	HEM	D	601	1	-	0/6/54/54	0/0/8/8
2	HEM	E	601	1	-	0/6/54/54	0/0/8/8
2	HEM	F	601	1	-	0/6/54/54	0/0/8/8
2	HEM	G	601	1	-	0/6/54/54	0/0/8/8
2	HEM	H	601	1,3	-	0/6/54/54	0/0/8/8
3	RIT	H	602	2	-	0/49/53/53	0/4/4/4
2	HEM	I	601	1	-	0/6/54/54	0/0/8/8
2	HEM	J	601	1	-	0/6/54/54	0/0/8/8
2	HEM	K	601	1	-	0/6/54/54	0/0/8/8
2	HEM	L	601	1	-	0/6/54/54	0/0/8/8

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	HEM	C3B-C2B	-4.22	1.34	1.40
2	H	601	HEM	C3C-C2C	-4.05	1.35	1.40
2	A	601	HEM	C3B-C2B	-3.96	1.35	1.40
2	B	601	HEM	C3B-C2B	-3.96	1.35	1.40
2	C	601	HEM	C3C-C2C	-3.95	1.35	1.40
2	D	601	HEM	C3C-C2C	-3.94	1.35	1.40
2	B	601	HEM	C3C-C2C	-3.92	1.35	1.40
2	K	601	HEM	C3C-C2C	-3.90	1.35	1.40
2	A	601	HEM	C3C-C2C	-3.89	1.35	1.40
2	J	601	HEM	C3B-C2B	-3.89	1.35	1.40
2	D	601	HEM	C3B-C2B	-3.88	1.35	1.40
2	J	601	HEM	C3C-C2C	-3.88	1.35	1.40
2	L	601	HEM	C3B-C2B	-3.87	1.35	1.40
2	F	601	HEM	C3C-C2C	-3.84	1.35	1.40
2	G	601	HEM	C3C-C2C	-3.84	1.35	1.40
2	G	601	HEM	C3B-C2B	-3.84	1.35	1.40
2	E	601	HEM	C3C-C2C	-3.81	1.35	1.40
2	E	601	HEM	C3B-C2B	-3.81	1.35	1.40
2	F	601	HEM	C3B-C2B	-3.80	1.35	1.40
2	I	601	HEM	C3C-C2C	-3.80	1.35	1.40
2	L	601	HEM	C3C-C2C	-3.79	1.35	1.40
2	C	601	HEM	C3B-C2B	-3.79	1.35	1.40
2	K	601	HEM	C3B-C2B	-3.78	1.35	1.40
2	I	601	HEM	C3B-C2B	-3.75	1.35	1.40
3	B	602	RIT	C4-N5	-2.76	1.29	1.34
3	H	602	RIT	C4-N5	-2.70	1.30	1.34
3	A	602	RIT	C4-N5	-2.67	1.30	1.34
2	H	601	HEM	C3B-CAB	3.82	1.55	1.47
2	F	601	HEM	C3B-CAB	3.90	1.55	1.47
2	C	601	HEM	C3B-CAB	3.90	1.55	1.47
2	K	601	HEM	C3B-CAB	3.90	1.55	1.47
2	L	601	HEM	C3B-CAB	3.94	1.55	1.47
2	D	601	HEM	C3C-CAC	3.94	1.55	1.47
2	J	601	HEM	C3B-CAB	3.95	1.55	1.47
2	A	601	HEM	C3C-CAC	3.95	1.55	1.47
2	I	601	HEM	C3B-CAB	3.96	1.55	1.47
2	D	601	HEM	C3B-CAB	3.96	1.55	1.47
2	K	601	HEM	C3C-CAC	3.97	1.55	1.47
2	A	601	HEM	C3B-CAB	3.97	1.55	1.47
2	L	601	HEM	C3C-CAC	3.99	1.55	1.47
2	J	601	HEM	C3C-CAC	3.99	1.55	1.47
2	E	601	HEM	C3B-CAB	3.99	1.55	1.47
2	C	601	HEM	C3C-CAC	4.00	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-CAB	4.01	1.55	1.47
2	G	601	HEM	C3B-CAB	4.03	1.55	1.47
2	E	601	HEM	C3C-CAC	4.03	1.55	1.47
2	G	601	HEM	C3C-CAC	4.05	1.55	1.47
2	F	601	HEM	C3C-CAC	4.06	1.55	1.47
2	B	601	HEM	C3C-CAC	4.07	1.55	1.47
2	I	601	HEM	C3C-CAC	4.14	1.56	1.47
2	H	601	HEM	C3C-CAC	4.23	1.56	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	CAA-CBA-CGA	-5.64	103.02	112.66
3	A	602	RIT	C77-C75-N74	-3.68	107.33	113.72
3	H	602	RIT	C77-C75-N74	-3.45	107.72	113.72
3	H	602	RIT	C26-C12-C13	-3.29	105.81	111.74
2	B	601	HEM	CAA-CBA-CGA	-2.50	108.39	112.66
2	H	601	HEM	CMD-C2D-C1D	-2.41	124.75	128.46
2	H	601	HEM	CAD-CBD-CGD	-2.40	108.56	112.66
2	D	601	HEM	CAA-CBA-CGA	-2.37	108.62	112.66
2	K	601	HEM	CMD-C2D-C1D	-2.26	124.98	128.46
2	A	601	HEM	CMD-C2D-C1D	-2.17	125.12	128.46
2	E	601	HEM	CMD-C2D-C1D	-2.14	125.18	128.46
3	A	602	RIT	C26-C12-C13	-2.12	107.92	111.74
2	F	601	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
2	B	601	HEM	CMD-C2D-C1D	-2.09	125.25	128.46
2	G	601	HEM	CMD-C2D-C1D	-2.05	125.31	128.46
2	I	601	HEM	CAA-CBA-CGA	-2.05	109.16	112.66
2	F	601	HEM	CAA-CBA-CGA	-2.03	109.20	112.66
2	D	601	HEM	CMD-C2D-C1D	-2.02	125.36	128.46
2	H	601	HEM	CAA-C2A-C3A	-2.01	123.26	129.00
2	B	601	HEM	CMB-C2B-C3B	2.01	128.62	124.89
2	D	601	HEM	C1D-C2D-C3D	2.04	108.42	107.00
2	D	601	HEM	CMB-C2B-C3B	2.06	128.72	124.89
2	J	601	HEM	CMB-C2B-C3B	2.07	128.74	124.89
2	A	601	HEM	CMC-C2C-C3C	2.08	128.75	124.89
2	D	601	HEM	CMC-C2C-C3C	2.08	128.76	124.89
2	J	601	HEM	CMC-C2C-C3C	2.08	128.76	124.89
2	G	601	HEM	CMB-C2B-C3B	2.09	128.77	124.89
2	C	601	HEM	CMB-C2B-C3B	2.09	128.78	124.89
2	K	601	HEM	CMC-C2C-C3C	2.11	128.80	124.89
2	E	601	HEM	CMB-C2B-C3B	2.12	128.82	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	HEM	CMC-C2C-C3C	2.13	128.85	124.89
2	A	601	HEM	CMB-C2B-C3B	2.14	128.87	124.89
2	B	601	HEM	CMC-C2C-C3C	2.15	128.89	124.89
2	L	601	HEM	CMB-C2B-C3B	2.16	128.90	124.89
2	L	601	HEM	CMC-C2C-C3C	2.19	128.95	124.89
2	I	601	HEM	CMB-C2B-C3B	2.20	128.97	124.89
2	K	601	HEM	CMB-C2B-C3B	2.21	129.00	124.89
2	E	601	HEM	CMC-C2C-C3C	2.28	129.12	124.89
2	F	601	HEM	CMB-C2B-C3B	2.33	129.21	124.89
2	H	601	HEM	CMB-C2B-C3B	2.36	129.26	124.89
2	H	601	HEM	CMC-C2C-C3C	2.39	129.33	124.89
3	H	602	RIT	C13-C12-N11	2.46	113.89	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	3	0
3	A	602	RIT	5	0
2	B	601	HEM	3	0
3	B	602	RIT	16	0
2	C	601	HEM	2	0
2	D	601	HEM	3	0
2	E	601	HEM	5	0
2	F	601	HEM	3	0
2	G	601	HEM	2	0
2	H	601	HEM	6	0
3	H	602	RIT	11	0
2	I	601	HEM	2	0
2	J	601	HEM	2	0
2	K	601	HEM	2	0
2	L	601	HEM	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	462/480 (96%)	-0.03	12 (2%) 56 52	31, 51, 83, 109	0
1	B	458/480 (95%)	0.26	18 (3%) 40 36	37, 63, 94, 129	0
1	C	469/480 (97%)	-0.03	11 (2%) 61 58	27, 45, 77, 111	0
1	D	459/480 (95%)	0.10	11 (2%) 59 56	35, 57, 85, 123	0
1	E	441/480 (91%)	0.96	67 (15%) 2 2	45, 100, 129, 141	0
1	F	456/480 (95%)	0.58	37 (8%) 13 9	55, 79, 111, 128	0
1	G	455/480 (94%)	0.02	5 (1%) 80 80	33, 56, 86, 109	0
1	H	459/480 (95%)	0.08	9 (1%) 65 63	40, 60, 84, 104	0
1	I	464/480 (96%)	0.09	11 (2%) 59 56	36, 54, 82, 123	0
1	J	458/480 (95%)	0.30	24 (5%) 28 24	31, 65, 94, 140	0
1	K	458/480 (95%)	0.09	12 (2%) 56 52	39, 60, 88, 133	0
1	L	448/480 (93%)	1.11	93 (20%) 1 1	64, 104, 135, 143	0
All	All	5487/5760 (95%)	0.29	310 (5%) 25 21	27, 63, 117, 143	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	257	LYS	6.2
1	L	377	CYS	6.2
1	E	338	VAL	6.1
1	J	265	GLN	6.0
1	E	489	VAL	5.9
1	J	27	THR	5.8
1	L	389	PRO	5.7
1	F	262	ASN	5.3
1	I	265	GLN	5.3
1	L	261	LEU	5.0
1	L	405	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	409	THR	4.9
1	F	469	GLU	4.8
1	F	407	TYR	4.7
1	F	473	PRO	4.7
1	E	326	ASP	4.7
1	L	491	LYS	4.6
1	E	490	LEU	4.6
1	E	459	LEU	4.5
1	J	266	LYS	4.5
1	L	465	LYS	4.5
1	E	352	GLN	4.5
1	E	290	LEU	4.4
1	J	492	VAL	4.4
1	L	387	PHE	4.4
1	L	464	PHE	4.4
1	F	416	PRO	4.3
1	E	258	LYS	4.3
1	L	486	LYS	4.3
1	L	276	ILE	4.3
1	L	419	PHE	4.2
1	E	327	VAL	4.1
1	C	168	LYS	4.1
1	L	275	MET	4.1
1	E	190	GLY	4.0
1	L	410	GLU	4.0
1	C	265	GLN	4.0
1	E	470	THR	4.0
1	F	51	LEU	4.0
1	D	266	LYS	3.9
1	L	216	LEU	3.9
1	K	266	LYS	3.9
1	B	425	SER	3.9
1	E	460	GLN	3.8
1	K	262	ASN	3.8
1	L	470	THR	3.8
1	L	271	PHE	3.8
1	D	27	THR	3.8
1	L	388	ILE	3.7
1	F	419	PHE	3.7
1	L	221	LEU	3.7
1	L	200	GLN	3.6
1	L	100	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	407	TYR	3.6
1	E	472	ILE	3.5
1	E	330	LYS	3.5
1	L	329	GLN	3.5
1	C	263	ASP	3.5
1	L	193	ILE	3.5
1	L	469	GLU	3.5
1	L	415	ARG	3.5
1	L	259	SER	3.5
1	L	493	ASP	3.4
1	E	471	GLN	3.4
1	E	341	ASN	3.4
1	E	443	GLY	3.4
1	L	468	LYS	3.3
1	E	354	GLU	3.3
1	K	267	HIS	3.3
1	J	199	PRO	3.3
1	I	168	LYS	3.3
1	I	285	GLU	3.3
1	E	99	TYR	3.3
1	H	387	PHE	3.3
1	L	467	CYS	3.3
1	E	369	VAL	3.3
1	J	262	ASN	3.2
1	B	27	THR	3.2
1	B	267	HIS	3.2
1	H	340	PRO	3.2
1	B	383	ILE	3.2
1	E	156	LEU	3.2
1	E	457	ARG	3.2
1	L	408	TRP	3.2
1	L	492	VAL	3.2
1	B	266	LYS	3.2
1	L	256	MET	3.2
1	L	164	ALA	3.2
1	L	168	LYS	3.1
1	D	424	ASP	3.1
1	F	264	LYS	3.1
1	L	35	ARG	3.1
1	L	236	LEU	3.1
1	L	45	PRO	3.1
1	C	285	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	220	PHE	3.1
1	B	269	LEU	3.1
1	F	53	TYR	3.1
1	L	101	VAL	3.1
1	F	459	LEU	3.1
1	A	267	HIS	3.0
1	F	266	LYS	3.0
1	E	337	ALA	3.0
1	J	425	SER	3.0
1	L	337	ALA	3.0
1	A	268	ARG	2.9
1	L	272	LEU	2.9
1	L	459	LEU	2.9
1	F	258	LYS	2.9
1	L	258	LYS	2.9
1	L	406	LYS	2.9
1	G	387	PHE	2.9
1	K	289	ALA	2.9
1	F	265	GLN	2.9
1	D	265	GLN	2.9
1	C	264	LYS	2.9
1	F	215	PHE	2.9
1	B	71	MET	2.9
1	F	100	SER	2.8
1	A	255	ARG	2.8
1	F	289	ALA	2.8
1	A	266	LYS	2.8
1	F	319	TYR	2.8
1	B	132	LEU	2.8
1	E	312	SER	2.8
1	E	256	MET	2.8
1	C	424	ASP	2.8
1	L	490	LEU	2.8
1	E	189	PHE	2.8
1	E	276	ILE	2.8
1	L	278	SER	2.8
1	J	264	LYS	2.8
1	I	266	LYS	2.8
1	E	261	LEU	2.8
1	J	200	GLN	2.8
1	J	468	LYS	2.7
1	L	429	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	166	LYS	2.7
1	L	197	ASN	2.7
1	A	168	LYS	2.7
1	K	276	ILE	2.7
1	L	70	LYS	2.7
1	J	489	VAL	2.7
1	L	417	GLU	2.7
1	B	265	GLN	2.7
1	L	327	VAL	2.7
1	E	200	GLN	2.7
1	F	163	GLU	2.7
1	E	140	GLY	2.7
1	E	419	PHE	2.7
1	J	407	TYR	2.6
1	E	309	THR	2.6
1	F	54	ARG	2.6
1	B	312	SER	2.6
1	J	469	GLU	2.6
1	G	261	LEU	2.6
1	L	392	SER	2.6
1	E	473	PRO	2.6
1	L	460	GLN	2.6
1	L	102	PHE	2.6
1	E	132	LEU	2.6
1	E	468	LYS	2.6
1	F	466	PRO	2.6
1	E	152	TYR	2.6
1	E	486	LYS	2.6
1	E	469	GLU	2.6
1	F	342	LYS	2.6
1	K	189	PHE	2.6
1	E	335	ILE	2.5
1	E	346	THR	2.5
1	A	341	ASN	2.5
1	K	279	GLN	2.5
1	L	170	VAL	2.5
1	E	348	ASP	2.5
1	F	464	PHE	2.5
1	E	349	ALA	2.5
1	E	116	SER	2.5
1	C	282	LYS	2.5
1	E	347	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	426	ILE	2.5
1	J	215	PHE	2.5
1	L	203	PHE	2.5
1	F	420	SER	2.5
1	F	385	GLY	2.5
1	L	321	LEU	2.5
1	A	289	ALA	2.5
1	J	261	LEU	2.5
1	E	262	ASN	2.4
1	H	290	LEU	2.4
1	G	168	LYS	2.4
1	J	444	MET	2.4
1	G	385	GLY	2.4
1	E	289	ALA	2.4
1	L	147	PRO	2.4
1	D	441	CYS	2.4
1	L	161	ARG	2.4
1	I	67	LYS	2.4
1	L	262	ASN	2.4
1	L	354	GLU	2.4
1	L	250	SER	2.4
1	H	289	ALA	2.4
1	F	261	LEU	2.4
1	F	468	LYS	2.4
1	B	262	ASN	2.4
1	L	254	ASN	2.4
1	B	426	ILE	2.4
1	J	267	HIS	2.4
1	E	55	GLN	2.4
1	J	441	CYS	2.4
1	A	280	ASN	2.4
1	L	260	ARG	2.3
1	L	338	VAL	2.3
1	J	387	PHE	2.3
1	H	312	SER	2.3
1	L	302	PHE	2.3
1	I	493	ASP	2.3
1	F	47	LEU	2.3
1	L	352	GLN	2.3
1	J	263	ASP	2.3
1	L	175	ILE	2.3
1	E	398	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	50	VAL	2.3
1	D	267	HIS	2.3
1	B	45	PRO	2.3
1	L	277	ASP	2.3
1	K	290	LEU	2.3
1	B	255	ARG	2.3
1	B	382	GLU	2.3
1	L	280	ASN	2.3
1	E	444	MET	2.3
1	A	387	PHE	2.3
1	K	265	GLN	2.3
1	L	165	GLU	2.3
1	L	93	VAL	2.2
1	F	408	TRP	2.2
1	E	295	LEU	2.2
1	E	97	GLU	2.2
1	L	158	ARG	2.2
1	H	262	ASN	2.2
1	E	148	ILE	2.2
1	E	368	PRO	2.2
1	E	275	MET	2.2
1	A	258	LYS	2.2
1	E	169	PRO	2.2
1	E	456	ILE	2.2
1	G	45	PRO	2.2
1	I	169	PRO	2.2
1	D	168	LYS	2.2
1	J	352	GLN	2.2
1	E	467	CYS	2.2
1	F	337	ALA	2.2
1	L	430	ILE	2.2
1	L	393	MET	2.2
1	L	167	GLY	2.2
1	L	435	GLY	2.2
1	F	290	LEU	2.2
1	I	45	PRO	2.2
1	L	34	LYS	2.2
1	L	466	PRO	2.2
1	L	75	TYR	2.2
1	D	51	LEU	2.1
1	H	424	ASP	2.1
1	L	290	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	262	ASN	2.1
1	A	494	SER	2.1
1	K	425	SER	2.1
1	E	101	VAL	2.1
1	D	263	ASP	2.1
1	E	464	PHE	2.1
1	C	422	LYS	2.1
1	E	257	LYS	2.1
1	E	441	CYS	2.1
1	F	219	LEU	2.1
1	E	433	PRO	2.1
1	D	264	LYS	2.1
1	H	266	LYS	2.1
1	L	328	GLN	2.1
1	D	139	SER	2.1
1	F	492	VAL	2.1
1	C	309	THR	2.1
1	I	261	LEU	2.1
1	L	160	LEU	2.1
1	E	96	LYS	2.1
1	F	406	LYS	2.1
1	H	41	PRO	2.1
1	L	152	TYR	2.1
1	L	325	PRO	2.1
1	L	131	SER	2.1
1	L	249	LEU	2.1
1	J	29	THR	2.1
1	A	281	SER	2.1
1	J	312	SER	2.1
1	B	387	PHE	2.1
1	B	310	THR	2.0
1	L	69	GLY	2.0
1	E	313	VAL	2.0
1	L	47	LEU	2.0
1	F	124	GLU	2.0
1	F	168	LYS	2.0
1	B	341	ASN	2.0
1	I	267	HIS	2.0
1	C	266	LYS	2.0
1	E	311	SER	2.0
1	E	371	ILE	2.0
1	C	215	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	32	LEU	2.0
1	K	469	GLU	2.0
1	J	311	SER	2.0
1	E	170	VAL	2.0
1	K	264	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	RIT	B	602	50/50	0.84	0.32	2.50	55,90,108,129	0
3	RIT	A	602	50/50	0.85	0.33	2.19	39,79,107,111	0
3	RIT	H	602	50/50	0.84	0.31	1.89	53,83,106,113	0
2	HEM	D	601	43/43	0.97	0.28	1.18	34,44,50,56	0
2	HEM	G	601	43/43	0.97	0.24	1.15	26,36,41,68	0
2	HEM	F	601	43/43	0.95	0.26	1.13	37,46,63,65	0
2	HEM	I	601	43/43	0.97	0.26	0.88	30,37,42,48	0
2	HEM	J	601	43/43	0.97	0.28	0.80	38,46,49,56	0
2	HEM	C	601	43/43	0.98	0.23	0.70	22,31,37,39	0
2	HEM	H	601	43/43	0.97	0.24	0.54	42,50,54,56	0
2	HEM	A	601	43/43	0.98	0.22	0.40	30,36,41,44	0
2	HEM	E	601	43/43	0.93	0.31	0.38	66,79,92,100	0
2	HEM	B	601	43/43	0.97	0.24	0.31	37,46,55,60	0
2	HEM	L	601	43/43	0.94	0.28	0.31	69,78,92,97	0
2	HEM	K	601	43/43	0.97	0.22	0.29	37,44,50,55	0

6.5 Other polymers

There are no such residues in this entry.