



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:06 AM GMT

PDB ID : 2P85
Title : Structure of Human Lung Cytochrome P450 2A13 with indole bound in two alternate conformations
Authors : Scott, E.E.; Stout, C.D.
Deposited on : 2007-03-21
Resolution : 2.35 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

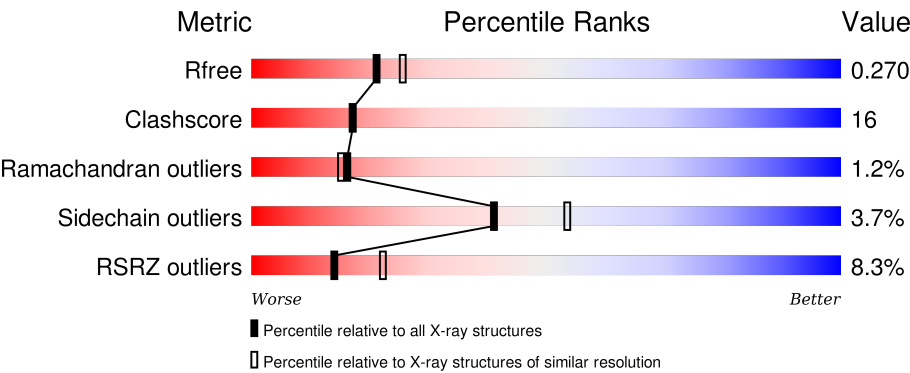
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	

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Mol	Chain	Length	Quality of chain
1	F	476	

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	IND	A	501[A]	-	-	-	X
3	IND	A	507[B]	-	-	-	X
3	IND	B	508[B]	-	-	X	-
3	IND	C	503[A]	-	-	-	X
3	IND	C	509[B]	-	-	-	X
3	IND	D	504[A]	-	-	-	X
3	IND	E	505[A]	-	-	-	X
3	IND	E	511[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23541 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 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	B	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	C	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	D	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	E	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	F	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	VAL	ENGINEERED	UNP Q16696
A	24	ALA	TRP	ENGINEERED	UNP Q16696
A	25	LYS	ARG	ENGINEERED	UNP Q16696
A	26	LYS	GLN	ENGINEERED	UNP Q16696
A	27	THR	ARG	ENGINEERED	UNP Q16696
A	28	SER	LYS	ENGINEERED	UNP Q16696
A	30	LYS	ARG	ENGINEERED	UNP Q16696
A	495	HIS	-	EXPRESSION TAG	UNP Q16696
A	496	HIS	-	EXPRESSION TAG	UNP Q16696
A	497	HIS	-	EXPRESSION TAG	UNP Q16696
A	498	HIS	-	EXPRESSION TAG	UNP Q16696
B	23	MET	VAL	ENGINEERED	UNP Q16696
B	24	ALA	TRP	ENGINEERED	UNP Q16696
B	25	LYS	ARG	ENGINEERED	UNP Q16696
B	26	LYS	GLN	ENGINEERED	UNP Q16696
B	27	THR	ARG	ENGINEERED	UNP Q16696
B	28	SER	LYS	ENGINEERED	UNP Q16696

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	LYS	ARG	ENGINEERED	UNP Q16696
B	495	HIS	-	EXPRESSION TAG	UNP Q16696
B	496	HIS	-	EXPRESSION TAG	UNP Q16696
B	497	HIS	-	EXPRESSION TAG	UNP Q16696
B	498	HIS	-	EXPRESSION TAG	UNP Q16696
C	23	MET	VAL	ENGINEERED	UNP Q16696
C	24	ALA	TRP	ENGINEERED	UNP Q16696
C	25	LYS	ARG	ENGINEERED	UNP Q16696
C	26	LYS	GLN	ENGINEERED	UNP Q16696
C	27	THR	ARG	ENGINEERED	UNP Q16696
C	28	SER	LYS	ENGINEERED	UNP Q16696
C	30	LYS	ARG	ENGINEERED	UNP Q16696
C	495	HIS	-	EXPRESSION TAG	UNP Q16696
C	496	HIS	-	EXPRESSION TAG	UNP Q16696
C	497	HIS	-	EXPRESSION TAG	UNP Q16696
C	498	HIS	-	EXPRESSION TAG	UNP Q16696
D	23	MET	VAL	ENGINEERED	UNP Q16696
D	24	ALA	TRP	ENGINEERED	UNP Q16696
D	25	LYS	ARG	ENGINEERED	UNP Q16696
D	26	LYS	GLN	ENGINEERED	UNP Q16696
D	27	THR	ARG	ENGINEERED	UNP Q16696
D	28	SER	LYS	ENGINEERED	UNP Q16696
D	30	LYS	ARG	ENGINEERED	UNP Q16696
D	495	HIS	-	EXPRESSION TAG	UNP Q16696
D	496	HIS	-	EXPRESSION TAG	UNP Q16696
D	497	HIS	-	EXPRESSION TAG	UNP Q16696
D	498	HIS	-	EXPRESSION TAG	UNP Q16696
E	23	MET	VAL	ENGINEERED	UNP Q16696
E	24	ALA	TRP	ENGINEERED	UNP Q16696
E	25	LYS	ARG	ENGINEERED	UNP Q16696
E	26	LYS	GLN	ENGINEERED	UNP Q16696
E	27	THR	ARG	ENGINEERED	UNP Q16696
E	28	SER	LYS	ENGINEERED	UNP Q16696
E	30	LYS	ARG	ENGINEERED	UNP Q16696
E	495	HIS	-	EXPRESSION TAG	UNP Q16696
E	496	HIS	-	EXPRESSION TAG	UNP Q16696
E	497	HIS	-	EXPRESSION TAG	UNP Q16696
E	498	HIS	-	EXPRESSION TAG	UNP Q16696
F	23	MET	VAL	ENGINEERED	UNP Q16696
F	24	ALA	TRP	ENGINEERED	UNP Q16696
F	25	LYS	ARG	ENGINEERED	UNP Q16696
F	26	LYS	GLN	ENGINEERED	UNP Q16696

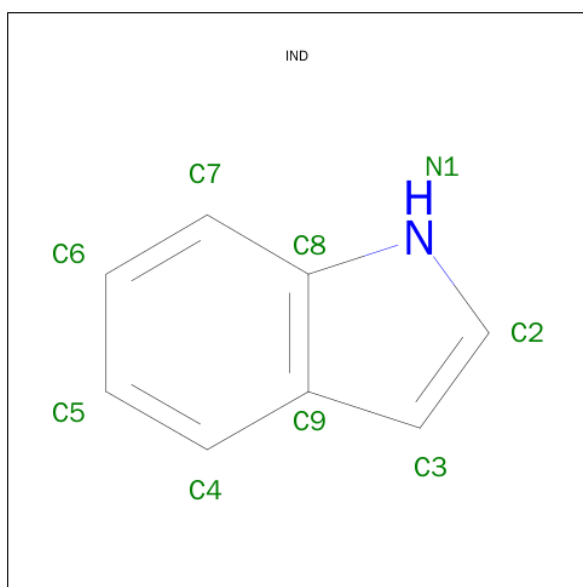
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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	THR	ARG	ENGINEERED	UNP Q16696
F	28	SER	LYS	ENGINEERED	UNP Q16696
F	30	LYS	ARG	ENGINEERED	UNP Q16696
F	495	HIS	-	EXPRESSION TAG	UNP Q16696
F	496	HIS	-	EXPRESSION TAG	UNP Q16696
F	497	HIS	-	EXPRESSION TAG	UNP Q16696
F	498	HIS	-	EXPRESSION TAG	UNP Q16696

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- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	1
			9	8	1		
3	A	1	Total	C	N	0	1
			9	8	1		
3	B	1	Total	C	N	0	1
			9	8	1		
3	B	1	Total	C	N	0	1
			9	8	1		
3	C	1	Total	C	N	0	1
			9	8	1		
3	C	1	Total	C	N	0	1
			9	8	1		
3	D	1	Total	C	N	0	1
			9	8	1		
3	D	1	Total	C	N	0	1
			9	8	1		
3	E	1	Total	C	N	0	1
			9	8	1		
3	E	1	Total	C	N	0	1
			9	8	1		
3	F	1	Total	C	N	0	1
			9	8	1		
3	F	1	Total	C	N	0	1
			9	8	1		

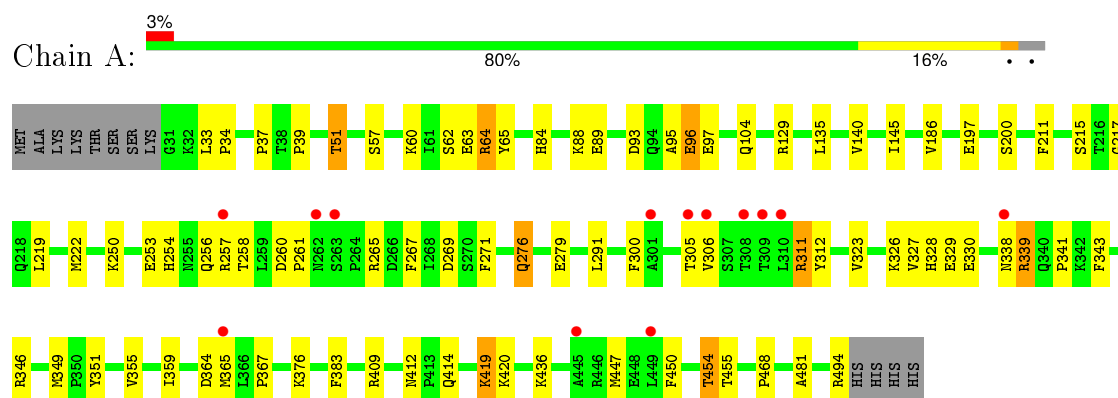
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total 161	O 161	0	1
4	B	75	Total 75	O 75	0	1
4	C	89	Total 89	O 89	0	1
4	D	96	Total 96	O 96	0	1
4	E	99	Total 99	O 99	0	1
4	F	77	Total 77	O 77	0	1

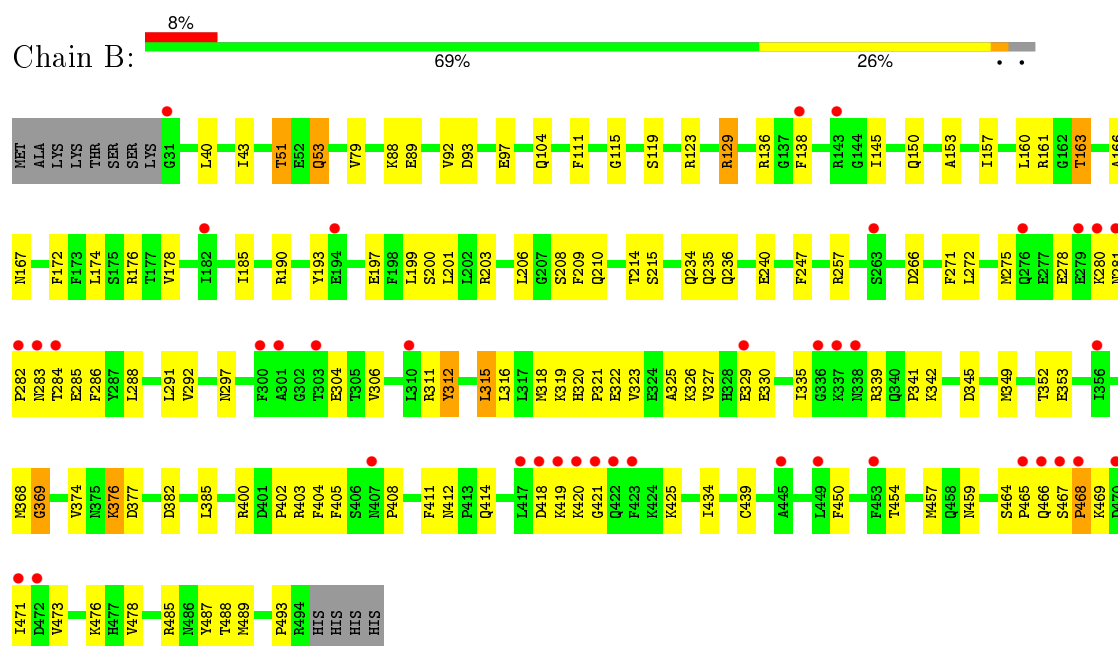
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 2A13

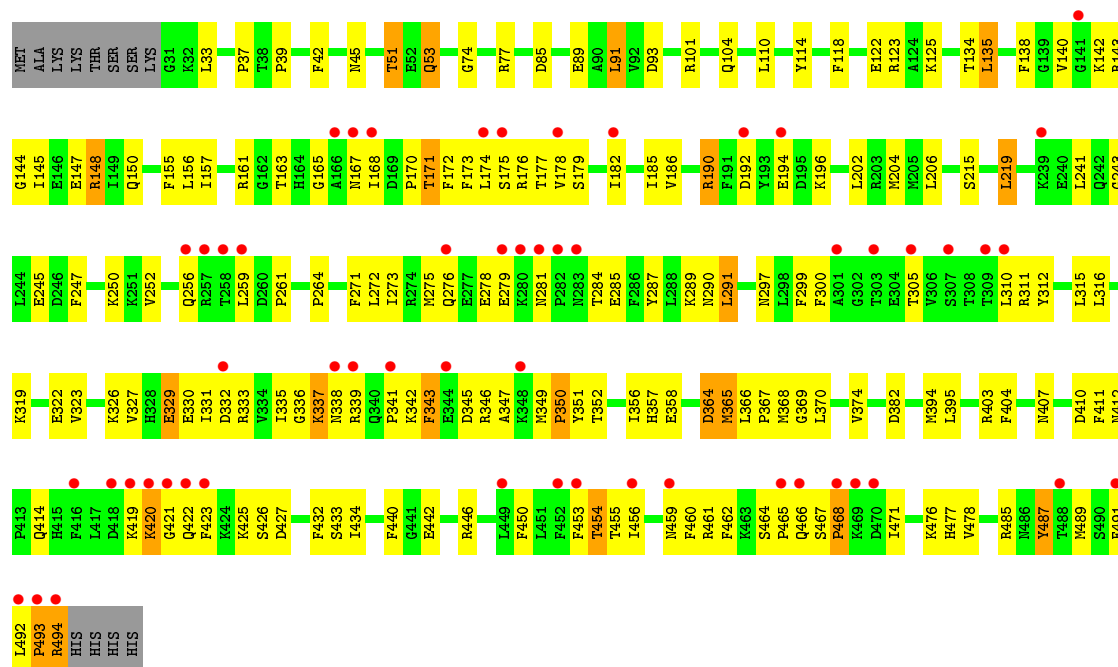


• Molecule 1: Cytochrome P450 2A13

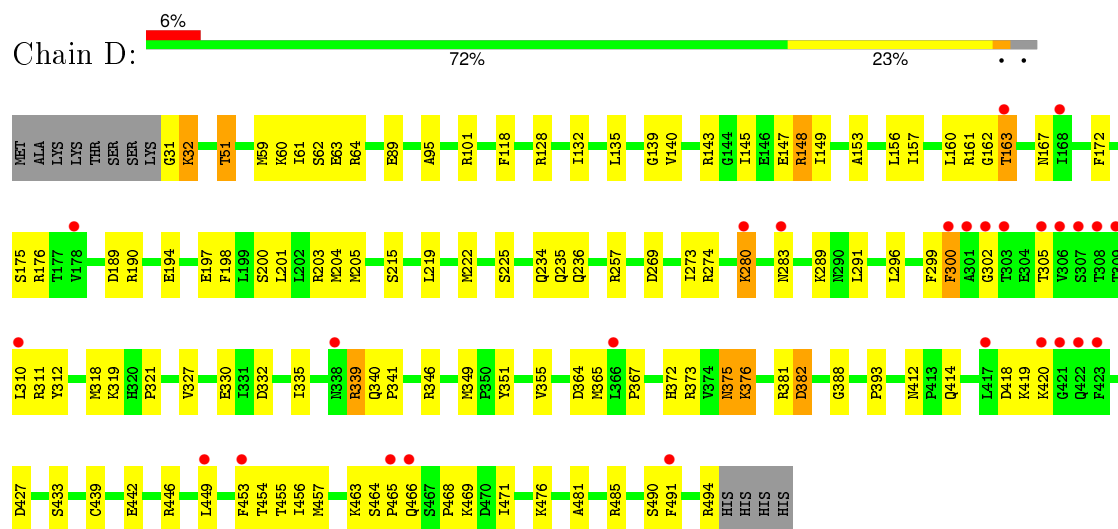


• Molecule 1: Cytochrome P450 2A13

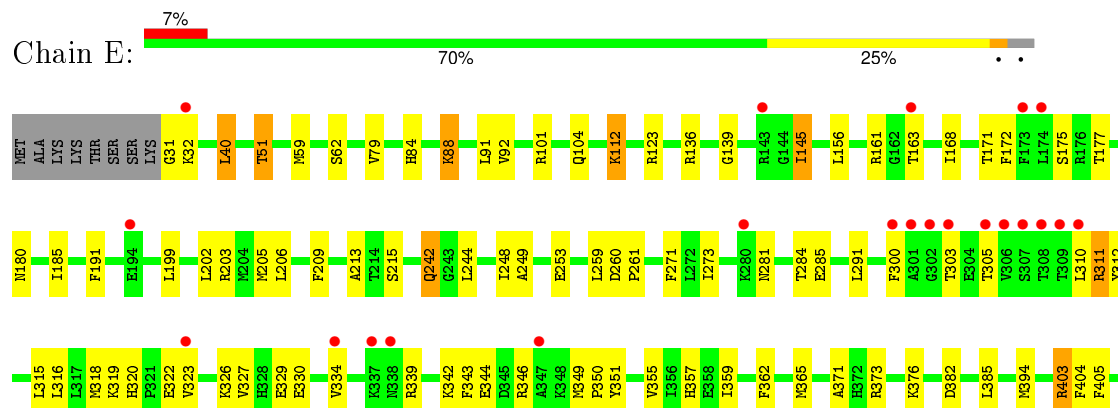


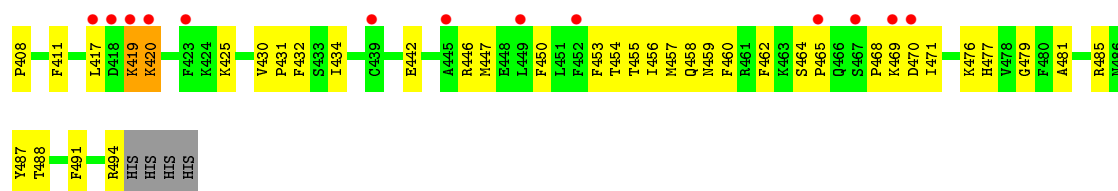


- Molecule 1: Cytochrome P450 2A13

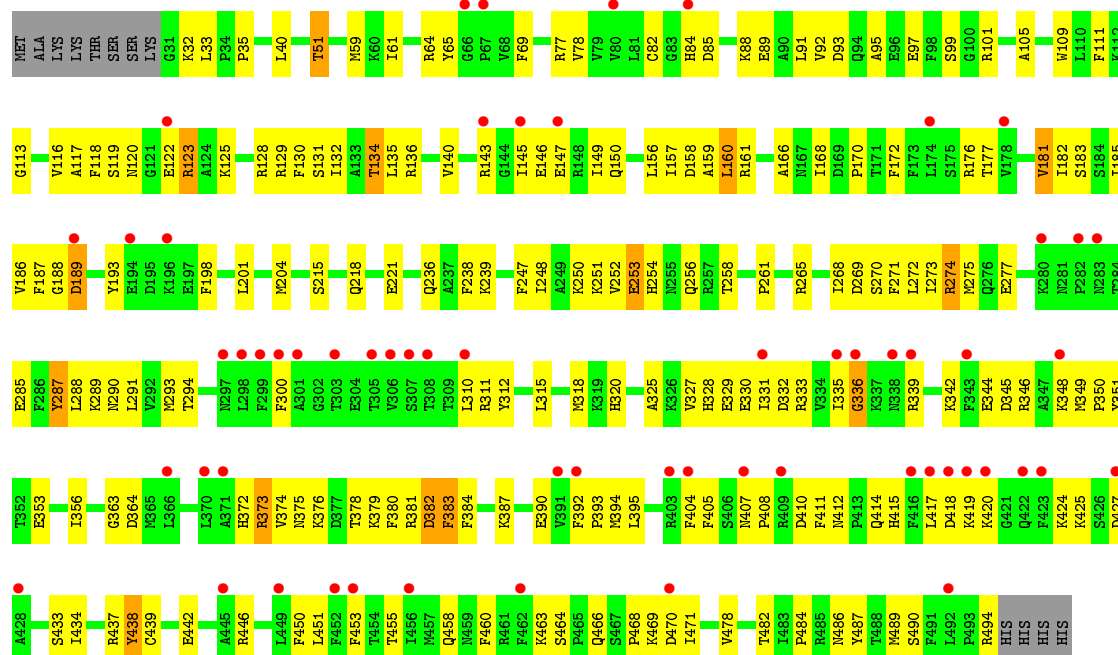


- Molecule 1: Cytochrome P450 2A13





• Molecule 1: Cytochrome P450 2A13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.32Å 110.28Å 142.00Å 90.00° 110.28° 90.00°	Depositor
Resolution (Å)	29.34 – 2.35 29.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.34-2.35) 96.9 (29.34-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.277 0.215 , 0.270	Depositor DCC
R_{free} test set	14041 reflections (10.98%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 198002 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23541	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IND, HEM

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	0/3860	0.68	1/5198 (0.0%)
1	B	0.45	0/3860	0.65	1/5198 (0.0%)
1	C	0.44	0/3860	0.64	3/5198 (0.1%)
1	D	0.46	0/3860	0.64	0/5198
1	E	0.44	0/3860	0.63	3/5198 (0.1%)
1	F	0.42	0/3860	0.61	0/5198
All	All	0.45	0/23160	0.64	8/31188 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLN	N-CA-C	-5.49	96.17	111.00
1	C	104	GLN	N-CA-C	-5.47	96.22	111.00
1	E	104	GLN	N-CA-C	-5.38	96.49	111.00
1	C	370	LEU	N-CA-C	-5.35	96.55	111.00
1	E	40	LEU	CA-CB-CG	-5.22	103.29	115.30
1	C	74	GLY	N-CA-C	-5.21	100.09	113.10
1	E	479	GLY	N-CA-C	-5.06	100.46	113.10
1	B	104	GLN	N-CA-C	-5.03	97.42	111.00

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	3763	0	3728	61	0
1	B	3763	0	3728	107	0
1	C	3763	0	3728	166	0
1	D	3763	0	3728	115	0
1	E	3763	0	3728	105	0
1	F	3763	0	3728	181	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
2	E	43	0	30	0	0
2	F	43	0	30	5	0
3	A	18	0	14	1	0
3	B	18	0	14	5	0
3	C	18	0	14	2	0
3	D	18	0	14	0	0
3	E	18	0	14	2	0
3	F	18	0	14	2	0
4	A	161	0	0	5	0
4	B	75	0	0	1	0
4	C	89	0	0	4	0
4	D	96	0	0	2	0
4	E	99	0	0	3	0
4	F	77	0	0	2	0
All	All	23541	0	22632	740	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 16.

All (740) 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:D:280:LYS:H	1:D:280:LYS:HE3	1.07	1.15
1:A:419:LYS:HD2	1:A:419:LYS:H	1.10	1.12
1:D:419:LYS:HD2	1:D:419:LYS:H	1.01	1.12
1:D:51:THR:HG23	1:D:215:SER:HB2	1.40	1.03
1:F:143:ARG:HH12	1:F:147:GLU:HB3	1.22	1.02
1:A:57:SER:HA	1:A:60:LYS:HE3	1.44	0.99
1:D:32:LYS:H	1:D:32:LYS:CE	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LYS:HD2	1:B:419:LYS:H	1.30	0.97
1:D:32:LYS:HE2	1:D:32:LYS:H	1.33	0.93
1:F:274:ARG:HB3	1:F:274:ARG:HH21	1.35	0.92
1:C:157:ILE:HG23	1:C:460:PHE:HE1	1.34	0.92
1:D:419:LYS:HD2	1:D:419:LYS:N	1.86	0.90
1:C:247:PHE:HD1	1:C:250:LYS:HE2	1.37	0.90
1:C:204:MET:CE	1:C:243:GLY:HA3	2.04	0.88
1:F:156:LEU:HD12	1:F:177:THR:OG1	1.73	0.87
1:A:420:LYS:HD2	1:A:420:LYS:H	1.40	0.87
1:D:280:LYS:N	1:D:280:LYS:HE3	1.91	0.85
1:F:143:ARG:NH1	1:F:147:GLU:HB3	1.91	0.85
1:E:242:GLN:HG2	4:E:1128:HOH:O	1.75	0.85
1:A:265:ARG:HD3	1:A:269:ASP:OD1	1.74	0.85
1:D:32:LYS:HE3	1:D:382:ASP:O	1.75	0.85
1:C:175:SER:HB2	1:C:202:LEU:HD11	1.59	0.84
1:C:247:PHE:CD1	1:C:250:LYS:HE2	2.13	0.84
1:C:144:GLY:O	1:C:147:GLU:HG2	1.78	0.83
1:E:450:PHE:O	1:E:454:THR:HG22	1.78	0.83
1:D:376:LYS:HB3	1:D:376:LYS:NZ	1.96	0.81
1:F:130:PHE:O	1:F:134:THR:HG22	1.80	0.81
1:D:468:PRO:HB2	1:D:469:LYS:HE3	1.62	0.81
1:F:420:LYS:HD2	1:F:420:LYS:N	1.96	0.80
1:B:330:GLU:OE1	1:B:352:THR:HG22	1.82	0.80
1:C:461:ARG:HE	1:C:494:ARG:HB2	1.47	0.79
1:B:53:GLN:NE2	1:B:478:VAL:HB	1.97	0.79
1:B:419:LYS:HD2	1:B:419:LYS:N	1.98	0.79
1:D:201:LEU:HD23	1:D:204:MET:HE3	1.63	0.78
1:C:450:PHE:O	1:C:454:THR:HB	1.82	0.78
1:C:247:PHE:O	1:C:250:LYS:HG2	1.83	0.78
1:E:31:GLY:O	1:E:32:LYS:HD2	1.84	0.78
1:F:201:LEU:HA	1:F:204:MET:HE3	1.64	0.77
1:C:335:ILE:HD13	1:C:341:PRO:HG3	1.64	0.77
1:B:53:GLN:HE21	1:B:478:VAL:HB	1.49	0.77
1:F:33:LEU:HD11	1:F:77:ARG:NH2	1.99	0.77
1:C:442:GLU:O	1:C:446:ARG:HG3	1.83	0.77
1:D:419:LYS:CD	1:D:419:LYS:H	1.86	0.77
1:A:254:HIS:O	1:A:257:ARG:HG2	1.84	0.77
1:A:419:LYS:N	1:A:419:LYS:HD2	1.94	0.77
1:F:442:GLU:O	1:F:446:ARG:HG3	1.85	0.77
1:E:156:LEU:HD21	1:E:456:ILE:HD11	1.67	0.76
1:D:219:LEU:HA	1:D:222:MET:HE3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ILE:HD12	1:C:173:PHE:CE2	2.21	0.75
1:B:172:PHE:O	1:B:176:ARG:HG3	1.87	0.75
1:C:315:LEU:HB2	1:C:487:TYR:HE2	1.50	0.75
1:B:197:GLU:O	1:B:200:SER:HB3	1.87	0.75
1:D:201:LEU:HD23	1:D:204:MET:CE	2.15	0.75
1:C:204:MET:HE1	1:C:243:GLY:HA3	1.70	0.74
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.53	0.74
1:F:130:PHE:CE2	1:F:274:ARG:HG3	2.22	0.73
1:C:315:LEU:HD13	1:C:487:TYR:CD2	2.23	0.73
1:F:274:ARG:HA	1:F:277:GLU:HG2	1.71	0.73
1:C:461:ARG:HH22	1:C:492:LEU:CD1	2.01	0.73
1:C:204:MET:HE2	1:C:243:GLY:HA3	1.71	0.72
1:C:297:ASN:HD22	3:C:503[A]:IND:HN1	1.35	0.72
1:F:32:LYS:H	1:F:384:PHE:HB3	1.53	0.72
1:E:405:PHE:O	1:E:408:PRO:HD3	1.89	0.72
1:D:60:LYS:O	1:D:63:GLU:HG2	1.90	0.71
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.90	0.71
1:C:460:PHE:HA	1:C:492:LEU:O	1.90	0.71
1:A:51:THR:HG23	1:A:215:SER:OG	1.90	0.71
1:B:209:PHE:CD2	1:B:304:GLU:HG2	2.26	0.71
1:E:92:VAL:HG23	1:E:434:ILE:HD12	1.72	0.70
1:C:172:PHE:HA	1:C:175:SER:OG	1.91	0.70
1:E:323:VAL:O	1:E:327:VAL:HG23	1.91	0.69
1:B:53:GLN:HE22	1:B:478:VAL:HG11	1.57	0.68
1:F:236:GLN:OE1	1:F:239:LYS:HE3	1.93	0.68
1:C:310:LEU:HD23	1:C:453:PHE:CE1	2.29	0.68
1:C:476:LYS:HE2	1:C:477:HIS:NE2	2.08	0.68
1:B:88:LYS:HG2	1:B:92:VAL:HG21	1.74	0.68
1:C:157:ILE:HG23	1:C:460:PHE:CE1	2.24	0.67
1:B:209:PHE:CE1	3:B:508[B]:IND:H2	2.30	0.67
1:F:254:HIS:O	1:F:258:THR:HG22	1.94	0.67
1:C:271:PHE:O	1:C:275:MET:HG3	1.95	0.67
1:D:219:LEU:HD12	1:D:222:MET:HE3	1.77	0.66
1:E:419:LYS:H	1:E:419:LYS:HZ2	1.44	0.66
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.09	0.66
1:F:310:LEU:HD23	1:F:453:PHE:CE1	2.30	0.66
1:C:51:THR:HG21	1:C:219:LEU:CD1	2.26	0.66
1:F:132:ILE:O	1:F:136:ARG:HG2	1.96	0.66
1:C:156:LEU:HD13	1:C:177:THR:OG1	1.96	0.66
1:E:355:VAL:O	1:E:359:ILE:HG13	1.95	0.66
1:F:88:LYS:HZ2	1:F:92:VAL:HG21	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:ARG:HH22	1:C:492:LEU:HD12	1.60	0.65
1:F:188:GLY:O	1:F:189:ASP:HB2	1.95	0.65
1:F:64:ARG:HD3	1:F:65:TYR:CE1	2.31	0.65
1:C:352:THR:O	1:C:356:ILE:HG13	1.97	0.65
1:F:486:ASN:N	1:F:486:ASN:HD22	1.94	0.65
1:E:357:HIS:CE1	1:E:446:ARG:HH22	2.15	0.65
1:D:176:ARG:HG3	1:D:198:PHE:CE2	2.31	0.65
1:A:419:LYS:CD	1:A:419:LYS:H	1.96	0.65
1:D:311:ARG:HH21	1:D:311:ARG:HG3	1.62	0.65
1:D:32:LYS:HE2	1:D:32:LYS:N	2.09	0.65
1:C:315:LEU:HD13	1:C:487:TYR:HD2	1.62	0.64
1:D:466:GLN:HE21	1:D:471:ILE:HG12	1.62	0.64
1:E:123:ARG:HA	1:E:285:GLU:HG3	1.80	0.64
1:F:328:HIS:O	1:F:331:ILE:HB	1.96	0.64
1:B:51:THR:HG22	1:B:215:SER:HB2	1.80	0.64
1:E:419:LYS:N	1:E:419:LYS:HD3	2.11	0.64
1:D:364:ASP:OD2	1:D:367:PRO:HB3	1.98	0.64
1:E:202:LEU:HD23	1:E:205:MET:CE	2.28	0.64
1:D:161:ARG:HH11	1:D:161:ARG:HG2	1.62	0.64
1:C:148:ARG:CA	1:C:148:ARG:HE	2.11	0.64
1:E:51:THR:HG23	1:E:215:SER:OG	1.98	0.64
1:C:461:ARG:HE	1:C:494:ARG:CB	2.11	0.63
1:A:420:LYS:N	1:A:420:LYS:HD2	2.12	0.63
1:B:419:LYS:CD	1:B:419:LYS:H	2.08	0.63
1:D:51:THR:CG2	1:D:215:SER:HB2	2.24	0.63
1:C:460:PHE:HD2	1:C:491:PHE:HB3	1.63	0.63
1:F:64:ARG:HH11	1:F:64:ARG:HG2	1.62	0.63
1:C:423:PHE:HE1	1:C:425:LYS:HG2	1.63	0.63
1:C:460:PHE:CD2	1:C:491:PHE:HB3	2.34	0.63
1:D:89:GLU:CD	1:D:381:ARG:HH11	2.02	0.63
1:B:51:THR:CG2	1:B:215:SER:HB2	2.29	0.63
1:B:342:LYS:HG3	1:B:345:ASP:OD1	1.99	0.63
1:B:400:ARG:HH11	1:B:400:ARG:HG3	1.64	0.62
1:F:330:GLU:OE2	1:F:350:PRO:HD2	1.99	0.62
1:F:248:ILE:O	1:F:252:VAL:HG23	1.98	0.62
1:F:88:LYS:HZ1	1:F:92:VAL:HG11	1.63	0.62
1:B:376:LYS:HD2	1:B:377:ASP:O	2.00	0.62
1:D:269:ASP:O	1:D:273:ILE:HG13	2.00	0.62
1:D:373:ARG:NH1	1:D:388:GLY:O	2.33	0.62
1:F:458:GLN:O	1:F:494:ARG:HD3	1.98	0.62
1:C:156:LEU:HD22	1:C:177:THR:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:HZ3	1:D:376:LYS:HB3	1.64	0.61
1:C:167:ASN:ND2	1:C:465:PRO:HB3	2.15	0.61
1:B:201:LEU:HD11	1:B:247:PHE:CZ	2.35	0.61
1:B:208:SER:N	1:B:240:GLU:OE2	2.33	0.61
1:D:442:GLU:O	1:D:446:ARG:HG3	2.00	0.61
1:F:157:ILE:HD11	1:F:455:THR:HG22	1.82	0.61
1:B:138:PHE:CZ	1:B:185:ILE:HA	2.35	0.61
1:F:327:VAL:O	1:F:331:ILE:HG13	2.01	0.61
1:D:319:LYS:O	1:D:321:PRO:HD3	2.00	0.61
1:D:51:THR:HG23	1:D:215:SER:CB	2.25	0.61
1:A:420:LYS:CD	1:A:420:LYS:H	2.12	0.61
1:A:51:THR:CG2	1:A:215:SER:OG	2.49	0.61
1:C:196:LYS:HE3	1:C:196:LYS:HA	1.83	0.60
1:B:174:LEU:HD12	1:B:311:ARG:HG2	1.83	0.60
1:F:265:ARG:HD3	1:F:269:ASP:OD1	2.01	0.60
1:B:53:GLN:HE22	1:B:478:VAL:CG1	2.14	0.60
1:F:136:ARG:HH11	1:F:136:ARG:HG3	1.65	0.60
1:F:51:THR:HG23	1:F:215:SER:HB2	1.82	0.60
1:F:270:SER:O	1:F:273:ILE:HB	2.01	0.60
1:B:450:PHE:O	1:B:454:THR:HG22	2.02	0.60
1:C:342:LYS:HD3	4:C:1031:HOH:O	2.01	0.60
1:B:402:PRO:C	1:B:404:PHE:H	2.05	0.59
1:B:53:GLN:NE2	1:B:478:VAL:CB	2.64	0.59
1:C:342:LYS:HG3	1:C:345:ASP:OD1	2.02	0.59
1:D:310:LEU:HD23	1:D:453:PHE:CE1	2.37	0.59
1:F:130:PHE:CE1	1:F:134:THR:HG21	2.38	0.59
1:F:130:PHE:O	1:F:134:THR:CG2	2.51	0.59
1:E:346:ARG:HB3	1:E:450:PHE:CE1	2.38	0.59
1:B:210:GLN:O	1:B:214:THR:HG23	2.02	0.59
1:B:89:GLU:HA	1:B:93:ASP:OD2	2.03	0.59
1:D:327:VAL:HG11	1:D:457:MET:CE	2.32	0.59
1:D:296:LEU:HD12	1:D:296:LEU:O	2.03	0.59
1:F:373:ARG:HH21	1:F:373:ARG:HB2	1.67	0.59
1:F:176:ARG:HD3	1:F:193:TYR:HA	1.85	0.58
1:E:101:ARG:O	1:E:373:ARG:HD2	2.03	0.58
1:C:425:LYS:HD3	1:C:426:SER:H	1.68	0.58
1:D:51:THR:O	1:D:215:SER:HA	2.03	0.58
1:D:332:ASP:OD2	1:D:494:ARG:NH2	2.37	0.58
1:D:341:PRO:HG2	1:D:454:THR:HG22	1.85	0.58
1:C:323:VAL:O	1:C:327:VAL:HG23	2.03	0.58
1:F:147:GLU:HA	1:F:150:GLN:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:VAL:HG23	1:B:374:VAL:O	2.03	0.58
1:D:219:LEU:HD12	1:D:222:MET:CE	2.34	0.57
1:F:433:SER:HB3	2:F:500:HEM:HBA1	1.86	0.57
1:E:51:THR:CG2	1:E:215:SER:OG	2.52	0.57
1:F:250:LYS:O	1:F:253:GLU:HG3	2.03	0.57
1:C:85:ASP:O	1:C:89:GLU:HG3	2.03	0.57
1:C:172:PHE:O	1:C:176:ARG:HG3	2.05	0.57
1:C:155:PHE:HD2	1:C:190:ARG:NH2	2.01	0.57
1:F:382:ASP:OD2	1:F:382:ASP:N	2.36	0.57
1:A:311:ARG:HG3	4:A:648:HOH:O	2.04	0.57
1:B:51:THR:HG23	1:B:215:SER:O	2.04	0.57
1:A:305:THR:HB	1:A:365:MET:HE1	1.86	0.57
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.69	0.57
1:E:156:LEU:CD2	1:E:456:ILE:HD11	2.33	0.57
1:C:51:THR:HG21	1:C:219:LEU:HD12	1.87	0.57
1:E:59:MET:O	1:E:62:SER:HB3	2.04	0.57
1:F:91:LEU:O	1:F:95:ALA:HA	2.05	0.57
1:C:174:LEU:HD22	1:C:310:LEU:HD13	1.87	0.57
1:C:89:GLU:O	1:C:93:ASP:HB2	2.05	0.57
1:A:341:PRO:HG2	1:A:454:THR:HG23	1.86	0.57
1:B:319:LYS:NZ	1:B:471:ILE:O	2.37	0.57
1:E:172:PHE:HA	1:E:175:SER:OG	2.04	0.57
1:F:161:ARG:HG2	1:F:161:ARG:HH11	1.69	0.57
1:C:134:THR:O	1:C:138:PHE:HD1	1.88	0.57
1:F:418:ASP:CA	1:F:424:LYS:HD2	2.34	0.56
1:A:219:LEU:HD12	1:A:222:MET:CE	2.35	0.56
1:F:330:GLU:CD	1:F:350:PRO:HD2	2.26	0.56
1:E:271:PHE:HB3	1:E:291:LEU:HD13	1.87	0.56
1:C:259:LEU:O	1:C:261:PRO:HD3	2.05	0.56
1:F:405:PHE:O	1:F:408:PRO:HD3	2.05	0.56
1:F:135:LEU:O	1:F:140:VAL:HB	2.05	0.56
1:D:32:LYS:N	1:D:32:LYS:CE	2.59	0.56
1:E:92:VAL:CG2	1:E:434:ILE:HD12	2.35	0.56
1:D:341:PRO:HB3	1:D:454:THR:HG21	1.86	0.56
1:A:409:ARG:HH21	1:A:409:ARG:HG3	1.69	0.56
1:E:112:LYS:HE3	4:E:758:HOH:O	2.03	0.56
1:D:148:ARG:HG3	1:D:148:ARG:HH21	1.70	0.56
1:E:205:MET:HE1	1:E:303:THR:HG21	1.87	0.56
1:F:251:LYS:NZ	1:F:251:LYS:HB3	2.19	0.56
1:F:88:LYS:NZ	1:F:92:VAL:HG21	2.21	0.56
1:B:400:ARG:NH1	1:B:400:ARG:HG3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HG2	1:C:333:ARG:HH21	1.69	0.56
1:F:130:PHE:HE2	1:F:274:ARG:HG3	1.67	0.56
1:F:105:ALA:HB3	1:F:221:GLU:OE2	2.05	0.56
1:D:375:ASN:HB3	4:D:613:HOH:O	2.05	0.56
1:B:167:ASN:OD1	1:B:488:THR:HB	2.06	0.56
1:E:261:PRO:HA	1:E:273:ILE:CD1	2.36	0.56
1:C:358:GLU:HA	1:C:358:GLU:OE1	2.05	0.55
1:F:335:ILE:HG23	1:F:339:ARG:NH2	2.22	0.55
1:F:331:ILE:HA	1:F:349:MET:HE3	1.87	0.55
1:A:253:GLU:HA	1:A:256:GLN:OE1	2.07	0.55
1:E:209:PHE:HE1	3:E:511[B]:IND:H3	1.72	0.55
1:E:403:ARG:HG3	1:E:404:PHE:CD2	2.41	0.55
1:C:168:ILE:HD12	1:C:173:PHE:HE2	1.69	0.55
1:B:319:LYS:HE3	1:B:468:PRO:O	2.06	0.55
1:C:461:ARG:HH22	1:C:492:LEU:HD13	1.71	0.55
1:F:172:PHE:O	1:F:176:ARG:HB2	2.06	0.55
1:F:149:ILE:HG21	1:F:451:LEU:HD12	1.88	0.55
1:E:419:LYS:O	1:E:420:LYS:HB2	2.06	0.55
1:F:325:ALA:O	1:F:328:HIS:HB2	2.06	0.55
1:F:128:ARG:O	1:F:132:ILE:HG13	2.06	0.55
1:C:172:PHE:HA	1:C:175:SER:HG	1.72	0.55
1:E:343:PHE:CE1	1:E:447:MET:HA	2.42	0.55
1:E:365:MET:O	1:E:481:ALA:HA	2.07	0.55
1:B:271:PHE:CG	1:B:291:LEU:HD23	2.42	0.55
1:C:37:PRO:HG2	1:C:45:ASN:ND2	2.22	0.55
1:F:372:HIS:HD2	1:F:393:PRO:HG2	1.72	0.55
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.07	0.54
1:F:318:MET:SD	1:F:464:SER:HB2	2.47	0.54
1:D:291:LEU:HD23	1:D:291:LEU:C	2.28	0.54
1:A:89:GLU:O	1:A:93:ASP:HB2	2.07	0.54
1:D:148:ARG:HG3	1:D:148:ARG:NH2	2.21	0.54
1:C:487:TYR:HD1	1:C:487:TYR:C	2.10	0.54
1:B:288:LEU:HD13	1:B:292:VAL:HG23	1.90	0.54
1:F:156:LEU:HD12	1:F:177:THR:CB	2.36	0.54
1:B:349:MET:HB3	1:B:352:THR:CG2	2.37	0.54
1:A:328:HIS:HB3	1:A:494:ARG:NH2	2.22	0.54
1:E:419:LYS:NZ	1:E:419:LYS:HB2	2.23	0.54
1:B:153:ALA:O	1:B:157:ILE:HG12	2.08	0.54
1:F:375:ASN:O	1:F:376:LYS:HG3	2.07	0.54
1:E:79:VAL:HG21	1:E:385:LEU:HD22	1.89	0.54
1:B:349:MET:HB3	1:B:352:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HA	1:D:222:MET:CE	2.37	0.54
1:C:315:LEU:HB2	1:C:487:TYR:CE2	2.38	0.54
1:C:487:TYR:CD1	1:C:487:TYR:C	2.81	0.54
1:D:469:LYS:CA	1:D:469:LYS:HE2	2.38	0.54
1:D:469:LYS:HE2	1:D:469:LYS:N	2.23	0.54
1:C:135:LEU:O	1:C:140:VAL:HG23	2.08	0.53
1:D:466:GLN:NE2	1:D:471:ILE:HG12	2.23	0.53
1:D:135:LEU:HD22	1:D:140:VAL:HG21	1.90	0.53
1:C:461:ARG:NH2	1:C:492:LEU:HD12	2.22	0.53
1:C:461:ARG:N	1:C:492:LEU:O	2.37	0.53
1:F:156:LEU:HD23	1:F:156:LEU:O	2.08	0.53
1:F:329:GLU:C	1:F:331:ILE:H	2.11	0.53
1:B:405:PHE:O	1:B:408:PRO:HD3	2.08	0.53
1:D:161:ARG:C	1:D:163:THR:H	2.12	0.53
1:B:325:ALA:O	1:B:329:GLU:HG3	2.08	0.53
1:F:123:ARG:HA	1:F:285:GLU:HG3	1.91	0.53
1:B:234:GLN:HG2	1:B:235:GLN:N	2.23	0.53
1:A:95:ALA:HB1	1:A:436:LYS:HG3	1.91	0.53
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.91	0.53
1:E:205:MET:CE	1:E:303:THR:HG21	2.39	0.53
1:D:160:LEU:HD22	1:D:491:PHE:CD2	2.44	0.53
1:F:414:GLN:NE2	1:F:417:LEU:HB2	2.23	0.53
1:E:322:GLU:O	1:E:326:LYS:HG3	2.10	0.52
1:F:97:GLU:O	1:F:374:VAL:HA	2.09	0.52
1:D:420:LYS:N	1:D:420:LYS:HD3	2.24	0.52
1:B:418:ASP:C	1:B:420:LYS:N	2.63	0.52
1:F:418:ASP:C	1:F:420:LYS:H	2.12	0.52
1:F:418:ASP:HA	1:F:424:LYS:HD2	1.90	0.52
1:E:271:PHE:CB	1:E:291:LEU:HD13	2.40	0.52
1:F:378:THR:HG22	1:F:379:LYS:N	2.24	0.52
1:D:89:GLU:OE2	1:D:381:ARG:NH1	2.42	0.52
1:E:457:MET:HG2	1:E:462:PHE:CZ	2.45	0.52
1:D:420:LYS:H	1:D:420:LYS:HD3	1.74	0.52
1:C:350:PRO:HG2	1:C:351:TYR:H	1.75	0.52
1:D:376:LYS:HZ2	1:D:376:LYS:HB3	1.74	0.52
1:F:335:ILE:O	1:F:335:ILE:HG22	2.10	0.52
1:F:95:ALA:O	1:F:99:SER:HB3	2.10	0.52
1:C:419:LYS:C	1:C:421:GLY:H	2.13	0.52
1:A:271:PHE:CG	1:A:291:LEU:HD13	2.44	0.52
1:B:476:LYS:HB2	1:B:485:ARG:HA	1.92	0.52
1:C:53:GLN:NE2	1:C:478:VAL:HB	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:THR:HG23	1:E:455:THR:H	1.75	0.52
1:F:342:LYS:HE2	1:F:344:GLU:CG	2.40	0.52
1:E:319:LYS:HB2	1:E:471:ILE:HG21	1.90	0.52
1:F:335:ILE:HD11	1:F:345:ASP:CB	2.40	0.52
1:D:161:ARG:HG2	1:D:161:ARG:NH1	2.24	0.52
1:C:148:ARG:HE	1:C:148:ARG:HA	1.73	0.52
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.91	0.51
1:E:344:GLU:HA	1:E:344:GLU:OE1	2.10	0.51
1:C:461:ARG:NH2	1:C:492:LEU:CD1	2.72	0.51
1:B:418:ASP:C	1:B:420:LYS:H	2.12	0.51
1:A:276:GLN:O	1:A:279:GLU:HG3	2.11	0.51
1:F:156:LEU:HD23	1:F:156:LEU:C	2.31	0.51
1:F:442:GLU:HG2	1:F:446:ARG:HD2	1.91	0.51
1:E:84:HIS:O	1:E:88:LYS:HB2	2.10	0.51
1:E:249:ALA:O	1:E:253:GLU:HG3	2.11	0.51
1:A:338:ASN:CG	1:A:339:ARG:H	2.14	0.51
1:E:31:GLY:C	1:E:32:LYS:HD2	2.31	0.51
1:C:466:GLN:HG2	1:C:467:SER:N	2.26	0.51
1:B:178:VAL:HG11	1:B:306:VAL:HB	1.93	0.51
1:B:53:GLN:NE2	1:B:478:VAL:CG1	2.73	0.51
1:D:128:ARG:O	1:D:132:ILE:HG13	2.11	0.51
1:C:276:GLN:O	1:C:279:GLU:HG3	2.11	0.51
2:A:500:HEM:C4D	3:A:507[B]:IND:H5	2.45	0.51
1:E:88:LYS:HD3	1:E:92:VAL:HB	1.93	0.51
1:B:138:PHE:CD2	1:B:138:PHE:O	2.64	0.51
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.25	0.51
1:F:486:ASN:ND2	1:F:486:ASN:N	2.58	0.51
1:B:320:HIS:O	1:B:323:VAL:HB	2.11	0.51
1:D:32:LYS:O	1:D:32:LYS:HE2	2.11	0.51
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.46	0.51
1:B:322:GLU:O	1:B:326:LYS:HG3	2.11	0.51
1:C:91:LEU:HB3	1:C:434:ILE:HG13	1.93	0.51
1:A:197:GLU:O	1:A:200:SER:HB3	2.11	0.51
1:D:341:PRO:CG	1:D:454:THR:HG22	2.41	0.50
1:A:64:ARG:HG3	1:A:65:TYR:CD2	2.46	0.50
1:F:182:ILE:O	1:F:186:VAL:HG13	2.11	0.50
1:F:158:ASP:HA	1:F:161:ARG:HD2	1.93	0.50
1:B:199:LEU:HD21	1:B:203:ARG:NH1	2.26	0.50
1:B:209:PHE:CD1	3:B:508[B]:IND:H2	2.46	0.50
1:E:323:VAL:HG13	1:E:351:TYR:OH	2.12	0.50
1:C:333:ARG:O	1:C:333:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ILE:HG23	1:D:339:ARG:NH1	2.26	0.50
1:C:170:PRO:CG	1:C:487:TYR:HE1	2.25	0.50
1:D:463:LYS:HB3	1:D:490:SER:OG	2.11	0.50
1:A:219:LEU:HD12	1:A:222:MET:HE3	1.93	0.50
1:E:476:LYS:HB2	1:E:485:ARG:HA	1.93	0.50
1:D:351:TYR:O	1:D:355:VAL:HG23	2.12	0.50
1:F:344:GLU:C	1:F:346:ARG:N	2.64	0.50
1:F:247:PHE:O	1:F:251:LYS:HG2	2.12	0.50
1:A:62:SER:C	1:A:64:ARG:H	2.14	0.50
1:C:305:THR:HG22	1:C:365:MET:HE1	1.93	0.50
1:F:274:ARG:HB3	1:F:274:ARG:NH2	2.14	0.49
1:E:319:LYS:HD2	1:E:468:PRO:O	2.12	0.49
1:E:199:LEU:HD21	1:E:203:ARG:HH11	1.76	0.49
1:E:316:LEU:HD13	1:E:411:PHE:CD2	2.47	0.49
1:B:275:MET:HG2	1:B:286:PHE:O	2.12	0.49
1:C:440:PHE:O	1:C:440:PHE:HD1	1.95	0.49
1:A:323:VAL:O	1:A:327:VAL:HG23	2.11	0.49
1:D:439:CYS:HB2	2:D:500:HEM:NA	2.26	0.49
1:E:425:LYS:HB2	4:E:773:HOH:O	2.12	0.49
1:D:197:GLU:O	1:D:200:SER:HB3	2.13	0.49
1:D:382:ASP:N	1:D:382:ASP:OD2	2.39	0.49
1:F:418:ASP:N	1:F:424:LYS:HD2	2.26	0.49
1:C:341:PRO:HG2	1:C:454:THR:HG23	1.94	0.49
1:A:219:LEU:HA	1:A:222:MET:HE2	1.92	0.49
1:C:252:VAL:O	1:C:256:GLN:HG3	2.11	0.49
1:F:329:GLU:C	1:F:331:ILE:N	2.65	0.49
1:F:289:LYS:HE2	4:F:1225:HOH:O	2.13	0.49
1:D:143:ARG:CZ	1:D:147:GLU:HG2	2.43	0.49
1:A:84:HIS:O	1:A:88:LYS:HB2	2.12	0.49
1:E:339:ARG:NH1	1:E:342:LYS:NZ	2.61	0.49
1:A:412:ASN:OD1	1:A:414:GLN:HB2	2.12	0.49
1:F:146:GLU:OE2	1:F:342:LYS:HB2	2.12	0.49
1:D:143:ARG:NH1	1:D:147:GLU:HG2	2.27	0.49
1:F:332:ASP:O	1:F:336:GLY:HA2	2.12	0.49
1:F:372:HIS:HE1	1:F:437:ARG:HB2	1.76	0.49
1:D:365:MET:O	1:D:481:ALA:HA	2.13	0.49
1:F:101:ARG:N	1:F:120:ASN:OD1	2.37	0.49
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.48	0.49
1:B:257:ARG:NH2	1:C:403:ARG:HB3	2.28	0.49
1:B:319:LYS:HG2	1:B:471:ILE:HD12	1.95	0.49
1:F:268:ILE:O	1:F:272:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LYS:HE2	1:D:469:LYS:HA	1.94	0.48
1:F:128:ARG:HG2	1:F:132:ILE:HD11	1.95	0.48
1:E:339:ARG:HH22	1:E:342:LYS:HG2	1.78	0.48
1:C:336:GLY:O	1:C:338:ASN:N	2.45	0.48
1:C:432:PHE:CD2	1:C:442:GLU:HG3	2.48	0.48
1:F:331:ILE:HG22	1:F:332:ASP:N	2.28	0.48
1:A:57:SER:HA	1:A:60:LYS:CE	2.29	0.48
1:E:163:THR:HG21	1:E:168:ILE:HD13	1.93	0.48
1:B:319:LYS:HE3	1:B:469:LYS:HA	1.96	0.48
1:E:271:PHE:CG	1:E:291:LEU:HD13	2.48	0.48
1:F:89:GLU:O	1:F:93:ASP:HB2	2.13	0.48
1:A:260:ASP:HB3	4:A:1238:HOH:O	2.14	0.48
1:D:449:LEU:O	1:D:453:PHE:HD1	1.96	0.48
1:A:33:LEU:HD22	1:A:33:LEU:N	2.28	0.48
1:C:461:ARG:HG2	1:C:461:ARG:HH11	1.79	0.48
1:F:158:ASP:O	1:F:161:ARG:HB2	2.14	0.48
1:A:37:PRO:HD3	1:A:65:TYR:CE2	2.48	0.48
1:E:465:PRO:HG3	1:E:488:THR:OG1	2.14	0.48
1:D:145:ILE:O	1:D:149:ILE:HG13	2.14	0.48
1:F:116:VAL:CG1	1:F:294:THR:HG23	2.44	0.48
1:E:244:LEU:O	1:E:248:ILE:HG12	2.14	0.48
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.95	0.48
1:E:454:THR:HG23	1:E:455:THR:N	2.29	0.48
1:F:330:GLU:HA	1:F:333:ARG:HH21	1.79	0.48
1:B:201:LEU:HD21	1:B:247:PHE:CG	2.48	0.48
1:B:467:SER:C	1:B:469:LYS:H	2.17	0.48
1:A:343:PHE:O	1:A:346:ARG:HG2	2.13	0.48
1:D:234:GLN:HG2	1:D:235:GLN:N	2.29	0.48
1:D:280:LYS:H	1:D:280:LYS:CE	1.99	0.48
1:C:271:PHE:CD2	1:C:291:LEU:HG	2.49	0.48
1:F:183:SER:O	1:F:187:PHE:HB2	2.13	0.48
1:C:327:VAL:O	1:C:331:ILE:HG13	2.14	0.48
1:B:403:ARG:HH21	1:B:403:ARG:HG3	1.79	0.48
1:E:320:HIS:HB3	1:E:323:VAL:HG23	1.94	0.48
1:D:32:LYS:CD	1:D:32:LYS:H	2.26	0.47
1:D:302:GLY:CA	2:D:500:HEM:HBC2	2.43	0.47
1:E:199:LEU:O	1:E:203:ARG:HB2	2.14	0.47
1:C:322:GLU:O	1:C:326:LYS:HG3	2.15	0.47
1:F:160:LEU:HB2	1:F:460:PHE:CE1	2.49	0.47
1:B:316:LEU:HD12	1:B:411:PHE:CG	2.49	0.47
1:E:419:LYS:H	1:E:419:LYS:HD3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:O	1:C:215:SER:HA	2.13	0.47
1:F:88:LYS:NZ	1:F:92:VAL:HG11	2.29	0.47
1:E:316:LEU:HD13	1:E:411:PHE:CE2	2.48	0.47
1:F:59:MET:HE2	1:F:82:CYS:SG	2.54	0.47
1:A:135:LEU:HB3	1:A:140:VAL:HG21	1.97	0.47
1:C:174:LEU:O	1:C:178:VAL:HG23	2.15	0.47
1:F:161:ARG:HG2	1:F:161:ARG:NH1	2.29	0.47
1:F:478:VAL:HG22	1:F:482:THR:HG23	1.97	0.47
1:D:418:ASP:C	1:D:418:ASP:OD2	2.52	0.47
1:E:156:LEU:HD22	1:E:177:THR:HG21	1.96	0.47
1:B:190:ARG:NH2	1:B:193:TYR:CE1	2.82	0.47
1:A:257:ARG:HG3	1:A:258:THR:HG23	1.97	0.47
1:C:272:LEU:O	1:C:275:MET:HB2	2.14	0.47
1:C:155:PHE:HD1	1:C:155:PHE:H	1.62	0.47
1:C:433:SER:CB	2:C:500:HEM:HBA1	2.45	0.47
1:E:311:ARG:HH21	1:E:311:ARG:HG3	1.80	0.47
1:F:274:ARG:CB	1:F:274:ARG:HH21	2.18	0.47
1:F:417:LEU:N	1:F:424:LYS:HG2	2.30	0.47
1:F:420:LYS:N	1:F:420:LYS:CD	2.70	0.47
1:B:376:LYS:O	1:B:377:ASP:C	2.52	0.47
1:F:393:PRO:O	1:F:395:LEU:N	2.46	0.47
1:C:91:LEU:HD12	1:C:91:LEU:HA	1.72	0.47
1:E:316:LEU:HD21	1:E:362:PHE:CE2	2.49	0.47
1:C:364:ASP:OD2	1:C:367:PRO:HB3	2.15	0.47
1:B:272:LEU:O	1:B:275:MET:HB2	2.15	0.47
1:F:288:LEU:O	1:F:291:LEU:HB3	2.15	0.47
1:E:458:GLN:C	1:E:459:ASN:HD22	2.18	0.47
1:F:287:TYR:CE1	1:F:290:ASN:ND2	2.83	0.47
1:F:356:ILE:CD1	1:F:450:PHE:HA	2.45	0.47
1:B:51:THR:O	1:B:215:SER:HA	2.15	0.47
1:C:155:PHE:CD1	1:C:155:PHE:N	2.83	0.47
1:F:251:LYS:HZ3	1:F:251:LYS:HB3	1.79	0.47
1:F:469:LYS:HE3	1:F:470:ASP:OD1	2.15	0.47
1:E:460:PHE:CD2	1:E:491:PHE:HB3	2.50	0.46
1:F:136:ARG:NH1	1:F:136:ARG:HG3	2.30	0.46
1:F:176:ARG:HG3	1:F:198:PHE:CE2	2.50	0.46
1:C:333:ARG:HG2	1:C:333:ARG:NH2	2.29	0.46
1:E:171:THR:OG1	1:E:311:ARG:HD3	2.15	0.46
1:A:355:VAL:O	1:A:359:ILE:HG13	2.14	0.46
1:C:206:LEU:HD12	4:C:1165:HOH:O	2.13	0.46
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:GLU:OE2	1:D:349:MET:HB3	2.15	0.46
1:E:329:GLU:OE2	1:E:330:GLU:N	2.47	0.46
1:C:165:GLY:HA2	1:C:491:PHE:O	2.16	0.46
1:D:172:PHE:HA	1:D:175:SER:OG	2.14	0.46
1:F:318:MET:HE1	1:F:489:MET:HB3	1.96	0.46
1:B:288:LEU:C	1:B:288:LEU:HD13	2.34	0.46
1:E:139:GLY:O	1:E:145:ILE:HB	2.15	0.46
1:D:346:ARG:HG2	1:D:346:ARG:HH21	1.80	0.46
1:E:326:LYS:HB2	1:E:351:TYR:CE2	2.49	0.46
1:F:88:LYS:HD3	1:F:92:VAL:HB	1.96	0.46
1:E:261:PRO:HA	1:E:273:ILE:HD11	1.97	0.46
1:E:469:LYS:HG3	1:E:470:ASP:N	2.30	0.46
1:A:34:PRO:HA	1:A:383:PHE:CE2	2.51	0.46
1:C:278:GLU:O	1:C:281:ASN:N	2.46	0.46
1:C:170:PRO:HG3	1:C:487:TYR:HE1	1.81	0.46
1:C:156:LEU:HD21	1:C:456:ILE:HD11	1.98	0.46
1:D:189:ASP:OD2	1:D:190:ARG:N	2.49	0.46
1:F:258:THR:HG23	1:F:265:ARG:HH22	1.80	0.46
1:C:332:ASP:OD1	1:C:337:LYS:HE3	2.15	0.46
1:B:402:PRO:C	1:B:404:PHE:N	2.69	0.46
1:C:281:ASN:O	1:C:284:THR:HG22	2.16	0.46
1:F:363:GLY:O	1:F:364:ASP:C	2.55	0.46
1:B:138:PHE:CE2	1:B:185:ILE:HA	2.51	0.45
1:B:320:HIS:N	1:B:321:PRO:HD3	2.31	0.45
1:E:432:PHE:CD2	1:E:442:GLU:HG3	2.50	0.45
1:E:343:PHE:O	1:E:346:ARG:HG2	2.16	0.45
1:D:201:LEU:CD2	1:D:204:MET:HE3	2.41	0.45
1:E:209:PHE:CE1	3:E:511[B]:IND:H3	2.51	0.45
1:C:468:PRO:HA	1:C:471:ILE:CD1	2.46	0.45
1:B:281:ASN:ND2	1:B:284:THR:N	2.64	0.45
1:B:138:PHE:HE1	1:B:266:ASP:HA	1.80	0.45
2:F:500:HEM:NA	3:F:512[B]:IND:H5	2.32	0.45
1:D:153:ALA:O	1:D:157:ILE:HG12	2.16	0.45
1:F:405:PHE:HD1	1:F:415:HIS:HB3	1.82	0.45
1:C:135:LEU:HG	1:C:140:VAL:HG21	1.96	0.45
1:B:327:VAL:HG11	1:B:457:MET:CE	2.45	0.45
1:C:339:ARG:HG3	1:C:339:ARG:O	2.16	0.45
1:D:32:LYS:CD	1:D:32:LYS:N	2.79	0.45
1:F:412:ASN:OD1	1:F:414:GLN:HB2	2.16	0.45
1:F:433:SER:CB	2:F:500:HEM:HBA1	2.46	0.45
1:E:305:THR:HG22	1:E:365:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:PHE:CD2	1:F:291:LEU:HD13	2.51	0.45
1:C:337:LYS:H	1:C:337:LYS:HD2	1.82	0.45
1:F:84:HIS:ND1	1:F:84:HIS:C	2.69	0.45
1:D:257:ARG:NE	1:D:257:ARG:HA	2.32	0.45
1:C:174:LEU:HD12	1:C:311:ARG:HG2	1.99	0.45
1:E:419:LYS:O	1:E:420:LYS:CB	2.65	0.45
1:F:176:ARG:CG	1:F:198:PHE:HE2	2.30	0.45
1:B:97:GLU:O	1:B:374:VAL:HA	2.17	0.45
1:E:459:ASN:HD22	1:E:459:ASN:N	2.12	0.45
1:A:330:GLU:OE2	1:A:349:MET:HB3	2.17	0.45
1:B:161:ARG:C	1:B:163:THR:H	2.20	0.45
1:C:155:PHE:HD1	1:C:155:PHE:N	2.14	0.45
1:F:469:LYS:HG3	1:F:470:ASP:OD1	2.17	0.45
1:F:438:TYR:CD2	1:F:438:TYR:C	2.90	0.45
1:F:156:LEU:O	1:F:159:ALA:HB3	2.17	0.45
1:F:335:ILE:O	1:F:336:GLY:C	2.55	0.45
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.99	0.45
1:B:79:VAL:HG21	1:B:385:LEU:HD22	1.99	0.45
1:F:342:LYS:N	1:F:345:ASP:OD2	2.44	0.45
1:F:373:ARG:HH22	1:F:390:GLU:HG2	1.80	0.45
1:F:315:LEU:HB2	1:F:487:TYR:CE2	2.52	0.45
1:C:182:ILE:O	1:C:186:VAL:HG22	2.17	0.45
1:C:369:GLY:HA2	1:C:395:LEU:HD12	1.98	0.45
1:B:92:VAL:CG2	1:B:434:ILE:HD12	2.46	0.45
1:F:61:ILE:O	1:F:61:ILE:HG22	2.17	0.45
1:F:166:ALA:O	1:F:168:ILE:HG23	2.17	0.45
1:F:92:VAL:HG23	1:F:434:ILE:HD12	1.98	0.44
1:F:380:PHE:O	1:F:381:ARG:C	2.55	0.44
1:C:264:PRO:HB3	1:C:273:ILE:HD12	1.99	0.44
1:D:318:MET:SD	1:D:464:SER:HB2	2.56	0.44
1:F:258:THR:CG2	1:F:265:ARG:HH22	2.29	0.44
1:F:318:MET:HE1	1:F:489:MET:CB	2.47	0.44
1:D:339:ARG:HH11	1:D:339:ARG:HG2	1.82	0.44
1:E:339:ARG:HH12	1:E:342:LYS:NZ	2.16	0.44
1:C:316:LEU:HD13	1:C:411:PHE:CE1	2.52	0.44
1:B:335:ILE:HG23	1:B:339:ARG:NH1	2.33	0.44
1:F:78:VAL:HG11	1:F:392:PHE:CD2	2.52	0.44
1:C:170:PRO:O	1:C:171:THR:C	2.56	0.44
1:E:351:TYR:O	1:E:355:VAL:HG23	2.17	0.44
1:C:271:PHE:HD2	1:C:275:MET:HG3	1.82	0.44
1:F:101:ARG:HG2	1:F:118:PHE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD12	1:B:43:ILE:HD11	1.99	0.44
1:C:420:LYS:O	1:C:422:GLN:HG2	2.17	0.44
1:E:180:ASN:OD1	1:E:191:PHE:HB2	2.17	0.44
1:C:271:PHE:CG	1:C:291:LEU:HG	2.51	0.44
1:F:176:ARG:HG2	1:F:198:PHE:HE2	1.82	0.44
1:E:403:ARG:HG3	1:E:404:PHE:CE2	2.52	0.44
1:B:412:ASN:OD1	1:B:414:GLN:CB	2.66	0.44
1:F:463:LYS:HB3	1:F:490:SER:HB2	1.98	0.44
1:F:458:GLN:HA	1:F:494:ARG:HH11	1.82	0.44
1:B:136:ARG:C	1:B:138:PHE:H	2.19	0.44
1:F:51:THR:O	1:F:215:SER:HA	2.18	0.44
1:F:145:ILE:HD11	1:F:181:VAL:HG13	1.98	0.44
1:D:156:LEU:CD2	1:D:456:ILE:HD11	2.48	0.44
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.18	0.44
1:C:101:ARG:HG2	1:C:118:PHE:HA	1.99	0.44
1:D:61:ILE:HG13	4:D:734:HOH:O	2.18	0.44
1:F:170:PRO:HG3	1:F:487:TYR:CE1	2.52	0.44
1:F:419:LYS:C	1:F:420:LYS:HD2	2.37	0.44
1:D:327:VAL:HG11	1:D:457:MET:HE1	2.00	0.44
1:F:168:ILE:HA	4:F:1119:HOH:O	2.18	0.44
1:C:343:PHE:O	1:C:346:ARG:HG2	2.18	0.44
1:F:404:PHE:N	1:F:404:PHE:CD1	2.86	0.44
1:B:115:GLY:O	1:B:119:SER:HB3	2.17	0.44
1:B:459:ASN:O	1:B:493:PRO:HA	2.18	0.44
1:F:201:LEU:CA	1:F:204:MET:HE3	2.40	0.43
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.53	0.43
1:E:315:LEU:HD13	1:E:487:TYR:CD2	2.53	0.43
1:E:318:MET:SD	1:E:464:SER:HB2	2.58	0.43
1:D:167:ASN:HD21	1:D:465:PRO:HD3	1.82	0.43
1:E:259:LEU:HD12	1:E:260:ASP:N	2.33	0.43
1:A:62:SER:O	1:A:64:ARG:N	2.51	0.43
1:F:469:LYS:HG3	1:F:470:ASP:N	2.31	0.43
1:A:326:LYS:HB2	1:A:351:TYR:CE2	2.54	0.43
1:F:84:HIS:ND1	1:F:85:ASP:N	2.67	0.43
1:B:464:SER:C	1:B:466:GLN:H	2.20	0.43
2:B:500:HEM:CHA	3:B:508[B]:IND:H5	2.47	0.43
1:D:161:ARG:C	1:D:163:THR:N	2.71	0.43
1:C:150:GLN:NE2	1:C:341:PRO:O	2.48	0.43
1:C:171:THR:HA	1:C:311:ARG:HD3	2.00	0.43
1:F:342:LYS:HE2	1:F:344:GLU:HG3	1.98	0.43
1:F:464:SER:C	1:F:466:GLN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:GLN:CG	1:C:467:SER:N	2.80	0.43
1:E:339:ARG:HH12	1:E:342:LYS:HZ3	1.65	0.43
1:F:468:PRO:HA	1:F:471:ILE:HD12	2.00	0.43
1:C:374:VAL:HG23	1:C:374:VAL:O	2.19	0.43
1:C:476:LYS:HB2	1:C:485:ARG:HA	2.01	0.43
1:C:148:ARG:NE	1:C:148:ARG:HA	2.33	0.43
1:C:155:PHE:CD2	1:C:190:ARG:NH2	2.84	0.43
1:A:343:PHE:CE1	1:A:447:MET:HA	2.53	0.43
1:A:97:GLU:HG3	1:A:376:LYS:HE2	2.00	0.43
1:C:493:PRO:HG2	1:C:494:ARG:H	1.84	0.43
1:C:272:LEU:HA	1:C:272:LEU:HD23	1.80	0.43
1:C:190:ARG:HG3	1:C:190:ARG:HH11	1.84	0.43
1:E:145:ILE:HD11	1:E:185:ILE:HD11	2.01	0.43
1:E:199:LEU:CD2	1:E:203:ARG:HH11	2.31	0.43
1:B:312:TYR:O	1:B:316:LEU:HD23	2.19	0.43
1:A:96:GLU:HG2	1:A:436:LYS:HE3	2.01	0.43
1:C:365:MET:O	1:C:366:LEU:HD23	2.19	0.43
1:D:139:GLY:O	1:D:145:ILE:HB	2.18	0.43
1:F:275:MET:HE3	1:F:287:TYR:HA	2.01	0.43
1:D:59:MET:O	1:D:62:SER:HB3	2.18	0.43
1:F:35:PRO:O	1:F:69:PHE:HB2	2.18	0.43
1:C:51:THR:HG23	1:C:215:SER:OG	2.19	0.43
1:D:172:PHE:O	1:D:176:ARG:HB2	2.19	0.43
1:D:305:THR:HG22	1:D:365:MET:CE	2.49	0.43
1:B:382:ASP:N	1:B:382:ASP:OD2	2.48	0.43
1:D:32:LYS:NZ	1:D:32:LYS:H	2.14	0.42
1:C:175:SER:HB2	1:C:202:LEU:CD1	2.40	0.42
1:C:419:LYS:O	1:C:421:GLY:N	2.52	0.42
1:C:440:PHE:O	1:C:440:PHE:CD1	2.72	0.42
1:D:157:ILE:HD11	1:D:455:THR:HG22	2.01	0.42
1:A:145:ILE:HD12	1:A:145:ILE:HA	1.85	0.42
1:D:31:GLY:HA2	1:D:32:LYS:HZ2	1.84	0.42
1:D:161:ARG:O	1:D:163:THR:N	2.53	0.42
1:F:350:PRO:HG2	1:F:351:TYR:H	1.84	0.42
1:F:116:VAL:HG13	1:F:117:ALA:N	2.35	0.42
1:C:110:LEU:HD22	1:C:241:LEU:HB3	2.00	0.42
1:C:357:HIS:CE1	1:C:446:ARG:NH2	2.87	0.42
1:B:150:GLN:NE2	1:B:341:PRO:O	2.43	0.42
1:B:368:MET:O	1:B:369:GLY:O	2.37	0.42
1:E:382:ASP:OD2	1:E:382:ASP:N	2.45	0.42
1:C:173:PHE:CD1	1:C:176:ARG:NH2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:MET:HE2	1:C:491:PHE:CE1	2.54	0.42
2:B:500:HEM:C1A	3:B:508[B]:IND:H5	2.54	0.42
1:E:351:TYR:HD1	1:E:417:LEU:HD11	1.84	0.42
1:F:88:LYS:HD3	1:F:88:LYS:O	2.20	0.42
1:D:311:ARG:NH2	1:D:311:ARG:HG3	2.32	0.42
1:E:319:LYS:HD3	1:E:471:ILE:HG22	2.01	0.42
1:C:403:ARG:HG3	4:C:912:HOH:O	2.18	0.42
1:C:433:SER:HB2	2:C:500:HEM:HBA1	2.01	0.42
1:C:264:PRO:HB3	1:C:273:ILE:CD1	2.48	0.42
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.50	0.42
1:C:122:GLU:O	1:C:125:LYS:HB3	2.18	0.42
1:C:192:ASP:OD1	1:C:194:GLU:HG2	2.19	0.42
1:C:168:ILE:HD11	1:C:491:PHE:CE1	2.55	0.42
3:B:508[B]:IND:H7	4:B:1242[B]:HOH:O	2.19	0.42
1:C:468:PRO:HA	1:C:471:ILE:HD12	2.01	0.42
1:E:351:TYR:CD1	1:E:417:LEU:HD11	2.54	0.42
1:C:467:SER:O	1:C:471:ILE:HG13	2.20	0.42
1:D:101:ARG:HG2	1:D:118:PHE:HA	2.02	0.42
1:D:203:ARG:HG2	1:D:203:ARG:HH11	1.83	0.42
1:C:175:SER:OG	1:C:202:LEU:HD21	2.19	0.42
1:C:454:THR:CG2	1:C:455:THR:N	2.83	0.42
1:B:376:LYS:C	1:B:376:LYS:HD2	2.40	0.42
1:A:339:ARG:HG2	1:A:339:ARG:HH21	1.85	0.42
1:D:302:GLY:HA3	2:D:500:HEM:HBC2	2.01	0.42
2:C:500:HEM:C1A	3:C:509[B]:IND:H5	2.55	0.42
1:F:353:GLU:HA	1:F:353:GLU:OE1	2.20	0.42
1:B:89:GLU:O	1:B:93:ASP:HB2	2.19	0.42
1:D:433:SER:CB	2:D:500:HEM:HBA1	2.49	0.42
1:C:287:TYR:CZ	1:C:290:ASN:ND2	2.88	0.42
1:F:311:ARG:NH1	1:F:484:PRO:HG2	2.34	0.42
1:C:145:ILE:HD11	1:C:185:ILE:HD11	2.01	0.42
1:D:372:HIS:CD2	1:D:393:PRO:HG2	2.55	0.42
1:C:175:SER:CB	1:C:202:LEU:HD21	2.50	0.42
1:A:365:MET:O	1:A:481:ALA:HA	2.20	0.42
1:A:88:LYS:HE3	4:A:949:HOH:O	2.20	0.42
1:E:281:ASN:HD22	1:E:284:THR:HB	1.84	0.42
1:A:211:PHE:CZ	1:A:217:GLY:HA2	2.55	0.42
1:F:111:PHE:HD2	1:F:293:MET:HB3	1.84	0.42
1:C:179:SER:OG	1:C:299:PHE:HE1	2.03	0.42
1:E:403:ARG:HD2	1:E:403:ARG:O	2.20	0.41
1:C:464:SER:C	1:C:466:GLN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ILE:HD13	1:F:185:ILE:HD11	2.02	0.41
1:F:109:TRP:CH2	1:F:238:PHE:HB3	2.55	0.41
1:E:310:LEU:HD23	1:E:453:PHE:CE1	2.55	0.41
1:C:368:MET:N	4:C:731:HOH:O	2.44	0.41
1:E:101:ARG:HD3	1:E:371:ALA:O	2.20	0.41
1:E:403:ARG:CG	1:E:403:ARG:O	2.68	0.41
1:F:464:SER:OG	1:F:466:GLN:HG2	2.19	0.41
1:A:346:ARG:HB3	1:A:450:PHE:CE2	2.55	0.41
1:E:459:ASN:ND2	1:E:459:ASN:N	2.68	0.41
1:C:382:ASP:N	1:C:382:ASP:OD2	2.45	0.41
1:C:114:TYR:CD2	1:C:289:LYS:HD2	2.55	0.41
1:C:114:TYR:CE2	1:C:289:LYS:HD2	2.55	0.41
1:C:462:PHE:CD2	1:C:489:MET:HE3	2.56	0.41
1:E:202:LEU:HD23	1:E:205:MET:HE1	2.01	0.41
1:B:201:LEU:HD11	1:B:247:PHE:CE2	2.55	0.41
1:C:331:ILE:HA	1:C:349:MET:HE1	2.02	0.41
4:A:989:HOH:O	1:D:64:ARG:HD2	2.20	0.41
1:F:407:ASN:HB3	1:F:410:ASP:HB2	2.00	0.41
1:C:461:ARG:NE	1:C:494:ARG:HB2	2.24	0.41
1:B:352:THR:HG23	1:B:353:GLU:N	2.35	0.41
1:E:456:ILE:O	1:E:460:PHE:HD1	2.04	0.41
1:B:281:ASN:OD1	1:B:282:PRO:HD2	2.20	0.41
1:B:161:ARG:C	1:B:163:THR:N	2.74	0.41
1:D:203:ARG:HG2	1:D:203:ARG:NH1	2.35	0.41
1:E:213:ALA:O	1:E:477:HIS:HB3	2.21	0.41
1:C:329:GLU:HG3	1:C:330:GLU:N	2.36	0.41
1:E:161:ARG:HH11	1:E:161:ARG:HG2	1.86	0.41
1:F:348:LYS:HD3	1:F:348:LYS:N	2.36	0.41
1:C:404:PHE:CD1	1:C:404:PHE:N	2.89	0.41
1:C:331:ILE:HA	1:C:349:MET:CE	2.51	0.41
1:C:407:ASN:HB3	1:C:410:ASP:OD2	2.20	0.41
1:F:160:LEU:N	1:F:160:LEU:CD1	2.83	0.41
1:F:111:PHE:CD2	1:F:293:MET:HB3	2.56	0.41
1:B:278:GLU:C	1:B:280:LYS:H	2.24	0.41
1:E:349:MET:N	1:E:350:PRO:CD	2.84	0.41
1:A:341:PRO:CG	1:A:454:THR:HG23	2.51	0.41
1:A:305:THR:OG1	1:A:306:VAL:N	2.54	0.41
1:F:256:GLN:HB2	1:F:272:LEU:HD21	2.03	0.41
1:D:145:ILE:HA	1:D:145:ILE:HD12	1.90	0.41
1:B:160:LEU:O	1:B:163:THR:HG22	2.21	0.41
1:B:335:ILE:HG23	1:B:339:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ARG:HG3	1:C:347:ALA:N	2.35	0.41
1:F:113:GLY:O	1:F:119:SER:HB3	2.20	0.41
1:E:430:VAL:N	1:E:431:PRO:CD	2.84	0.41
1:D:289:LYS:HE3	1:D:289:LYS:HB2	1.84	0.41
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.86	0.41
1:D:300:PHE:HD2	1:D:300:PHE:O	2.03	0.41
1:B:318:MET:HE1	1:B:489:MET:HB3	2.03	0.41
1:F:418:ASP:C	1:F:420:LYS:N	2.72	0.41
1:F:201:LEU:HD23	1:F:204:MET:CE	2.51	0.41
1:F:439:CYS:HB2	2:F:500:HEM:NA	2.35	0.41
1:D:365:MET:HE2	1:D:365:MET:HB3	1.86	0.41
1:A:351:TYR:O	1:A:355:VAL:HG23	2.21	0.41
1:B:43:ILE:HD13	1:F:40:LEU:HD11	2.03	0.41
1:F:122:GLU:O	1:F:125:LYS:N	2.54	0.41
1:F:332:ASP:O	1:F:336:GLY:CA	2.70	0.40
1:C:161:ARG:C	1:C:163:THR:H	2.24	0.40
1:B:315:LEU:HD13	1:B:487:TYR:CE2	2.56	0.40
1:F:218:GLN:HA	1:F:218:GLN:NE2	2.35	0.40
1:A:454:THR:CG2	1:A:455:THR:N	2.83	0.40
1:F:375:ASN:O	1:F:387:LYS:HG3	2.22	0.40
1:B:368:MET:C	1:B:369:GLY:O	2.59	0.40
1:B:111:PHE:CE2	1:B:297:ASN:ND2	2.90	0.40
1:A:265:ARG:HD2	4:A:1238:HOH:O	2.21	0.40
1:D:176:ARG:HG3	1:D:198:PHE:HE2	1.84	0.40
2:F:500:HEM:C1A	3:F:512[B]:IND:H5	2.56	0.40
1:C:319:LYS:HA	1:C:471:ILE:HD12	2.04	0.40
1:C:245:GLU:O	1:C:245:GLU:HG2	2.21	0.40
1:E:156:LEU:HD13	1:E:177:THR:OG1	2.20	0.40
1:F:438:TYR:CD2	1:F:438:TYR:O	2.74	0.40
1:F:320:HIS:CD2	1:F:411:PHE:CD2	3.10	0.40
1:A:364:ASP:O	1:A:367:PRO:HD3	2.22	0.40
1:D:412:ASN:OD1	1:D:414:GLN:HG2	2.22	0.40
1:F:332:ASP:HA	1:F:336:GLY:HA2	2.03	0.40
1:F:373:ARG:HB2	1:F:373:ARG:NH2	2.32	0.40
1:E:330:GLU:O	1:E:334:VAL:HG23	2.22	0.40
1:D:205:MET:HE2	1:D:299:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

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	462/476 (97%)	434 (94%)	26 (6%)	2 (0%)	39	46
1	B	462/476 (97%)	416 (90%)	40 (9%)	6 (1%)	15	13
1	C	462/476 (97%)	403 (87%)	47 (10%)	12 (3%)	7	4
1	D	462/476 (97%)	441 (96%)	19 (4%)	2 (0%)	39	46
1	E	462/476 (97%)	424 (92%)	36 (8%)	2 (0%)	39	46
1	F	462/476 (97%)	407 (88%)	47 (10%)	8 (2%)	11	9
All	All	2772/2856 (97%)	2525 (91%)	215 (8%)	32 (1%)	16	15

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	C	142	LYS
1	C	171	THR
1	C	337	LYS
1	E	420	LYS
1	B	369	GLY
1	C	394	MET
1	C	459	ASN
1	C	493	PRO
1	F	189	ASP
1	F	425	LYS
1	B	425	LYS
1	C	364	ASP
1	F	123	ARG
1	F	383	PHE
1	A	261	PRO
1	C	420	LYS
1	E	394	MET
1	F	394	MET
1	B	166	ALA

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Mol	Chain	Res	Type
1	B	468	PRO
1	C	42	PHE
1	C	190	ARG
1	F	261	PRO
1	B	421	GLY
1	D	95	ALA
1	C	350	PRO
1	C	468	PRO
1	F	181	VAL
1	F	336	GLY
1	D	162	GLY
1	B	465	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	408/419 (97%)	394 (97%)	14 (3%)	44	57
1	B	408/419 (97%)	397 (97%)	11 (3%)	52	67
1	C	408/419 (97%)	390 (96%)	18 (4%)	35	44
1	D	408/419 (97%)	391 (96%)	17 (4%)	36	46
1	E	408/419 (97%)	392 (96%)	16 (4%)	39	51
1	F	408/419 (97%)	393 (96%)	15 (4%)	41	53
All	All	2448/2514 (97%)	2357 (96%)	91 (4%)	41	53

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	51	THR
1	A	64	ARG
1	A	96	GLU
1	A	250	LYS
1	A	276	GLN

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Mol	Chain	Res	Type
1	A	300	PHE
1	A	311	ARG
1	A	312	TYR
1	A	329	GLU
1	A	339	ARG
1	A	419	LYS
1	A	454	THR
1	A	468	PRO
1	B	51	THR
1	B	53	GLN
1	B	129	ARG
1	B	163	THR
1	B	206	LEU
1	B	236	GLN
1	B	283	ASN
1	B	312	TYR
1	B	315	LEU
1	B	376	LYS
1	B	473	VAL
1	C	39	PRO
1	C	51	THR
1	C	53	GLN
1	C	91	LEU
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	219	LEU
1	C	291	LEU
1	C	300	PHE
1	C	312	TYR
1	C	329	GLU
1	C	343	PHE
1	C	365	MET
1	C	427	ASP
1	C	454	THR
1	C	487	TYR
1	C	494	ARG
1	D	32	LYS
1	D	51	THR
1	D	148	ARG
1	D	163	THR
1	D	194	GLU

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Mol	Chain	Res	Type
1	D	225	SER
1	D	274	ARG
1	D	280	LYS
1	D	283	ASN
1	D	300	PHE
1	D	312	TYR
1	D	339	ARG
1	D	340	GLN
1	D	375	ASN
1	D	376	LYS
1	D	382	ASP
1	D	427	ASP
1	E	40	LEU
1	E	51	THR
1	E	88	LYS
1	E	91	LEU
1	E	112	LYS
1	E	136	ARG
1	E	145	ILE
1	E	206	LEU
1	E	242	GLN
1	E	300	PHE
1	E	311	ARG
1	E	312	TYR
1	E	376	LYS
1	E	403	ARG
1	E	419	LYS
1	E	494	ARG
1	F	51	THR
1	F	129	ARG
1	F	131	SER
1	F	134	THR
1	F	160	LEU
1	F	253	GLU
1	F	274	ARG
1	F	287	TYR
1	F	300	PHE
1	F	312	TYR
1	F	373	ARG
1	F	382	ASP
1	F	383	PHE
1	F	427	ASP

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Mol	Chain	Res	Type
1	F	438	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	283	ASN
1	B	210	GLN
1	B	255	ASN
1	B	276	GLN
1	B	283	ASN
1	B	297	ASN
1	B	466	GLN
1	C	254	HIS
1	C	297	ASN
1	C	328	HIS
1	C	486	ASN
1	D	276	GLN
1	D	283	ASN
1	D	297	ASN
1	D	458	GLN
1	D	466	GLN
1	E	236	GLN
1	E	242	GLN
1	E	276	GLN
1	E	340	GLN
1	E	458	GLN
1	E	459	ASN
1	E	486	ASN
1	F	276	GLN
1	F	320	HIS
1	F	340	GLN
1	F	486	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 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	500	1	30,50,50	3.64	13 (43%)	24,82,82	2.72	9 (37%)
3	IND	A	501[A]	-	8,10,10	1.16	0	9,13,13	0.55	0
3	IND	A	507[B]	-	8,10,10	0.82	0	9,13,13	0.58	0
2	HEM	B	500	1	30,50,50	3.67	14 (46%)	24,82,82	2.65	9 (37%)
3	IND	B	502[A]	-	8,10,10	1.10	1 (12%)	9,13,13	0.51	0
3	IND	B	508[B]	-	8,10,10	0.93	0	9,13,13	0.63	0
2	HEM	C	500	1	30,50,50	3.67	13 (43%)	24,82,82	2.70	9 (37%)
3	IND	C	503[A]	-	8,10,10	1.18	1 (12%)	9,13,13	0.53	0
3	IND	C	509[B]	-	8,10,10	0.87	0	9,13,13	0.62	0
2	HEM	D	500	1	30,50,50	3.97	14 (46%)	24,82,82	2.72	9 (37%)
3	IND	D	504[A]	-	8,10,10	1.08	1 (12%)	9,13,13	0.51	0
3	IND	D	510[B]	-	8,10,10	0.86	0	9,13,13	0.59	0
2	HEM	E	500	1	30,50,50	3.70	14 (46%)	24,82,82	2.67	9 (37%)
3	IND	E	505[A]	-	8,10,10	1.11	1 (12%)	9,13,13	0.51	0
3	IND	E	511[B]	-	8,10,10	0.97	0	9,13,13	0.64	0
2	HEM	F	500	1	30,50,50	3.39	13 (43%)	24,82,82	2.68	9 (37%)
3	IND	F	506[A]	-	8,10,10	1.13	1 (12%)	9,13,13	0.50	0
3	IND	F	512[B]	-	8,10,10	0.69	0	9,13,13	0.64	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
2	HEM	A	500	1	-	0/10/54/54	0/0/8/8
3	IND	A	501[A]	-	-	0/0/0/0	0/2/2/2
3	IND	A	507[B]	-	-	0/0/0/0	0/2/2/2
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	IND	B	502[A]	-	-	0/0/0/0	0/2/2/2
3	IND	B	508[B]	-	-	0/0/0/0	0/2/2/2
2	HEM	C	500	1	-	0/10/54/54	0/0/8/8
3	IND	C	503[A]	-	-	0/0/0/0	0/2/2/2
3	IND	C	509[B]	-	-	0/0/0/0	0/2/2/2
2	HEM	D	500	1	-	0/10/54/54	0/0/8/8
3	IND	D	504[A]	-	-	0/0/0/0	0/2/2/2
3	IND	D	510[B]	-	-	0/0/0/0	0/2/2/2
2	HEM	E	500	1	-	0/10/54/54	0/0/8/8
3	IND	E	505[A]	-	-	0/0/0/0	0/2/2/2
3	IND	E	511[B]	-	-	0/0/0/0	0/2/2/2
2	HEM	F	500	1	-	0/10/54/54	0/0/8/8
3	IND	F	506[A]	-	-	0/0/0/0	0/2/2/2
3	IND	F	512[B]	-	-	0/0/0/0	0/2/2/2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3B-C4B	-11.56	1.41	1.51
2	E	500	HEM	C3B-C4B	-10.29	1.42	1.51
2	C	500	HEM	C3B-C4B	-9.91	1.43	1.51
2	B	500	HEM	C3B-C4B	-9.79	1.43	1.51
2	A	500	HEM	C3B-C4B	-9.48	1.43	1.51
2	D	500	HEM	C3D-C4D	-9.17	1.39	1.51
2	A	500	HEM	C3D-C4D	-8.89	1.40	1.51
2	C	500	HEM	C3D-C4D	-7.81	1.41	1.51
2	D	500	HEM	C2C-C1C	-7.74	1.37	1.52
2	E	500	HEM	C3D-C4D	-7.74	1.41	1.51
2	B	500	HEM	C3D-C4D	-7.73	1.41	1.51
2	F	500	HEM	C3B-C4B	-7.68	1.45	1.51
2	B	500	HEM	C3C-CAC	-7.61	1.37	1.51
2	F	500	HEM	C3D-C4D	-7.42	1.42	1.51
2	F	500	HEM	C2C-C1C	-7.42	1.38	1.52
2	C	500	HEM	C2C-C1C	-7.38	1.38	1.52
2	F	500	HEM	C3C-CAC	-7.37	1.37	1.51
2	E	500	HEM	C2C-C1C	-7.32	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3C-CAC	-7.26	1.37	1.51
2	C	500	HEM	C3C-CAC	-7.21	1.37	1.51
2	E	500	HEM	C3C-CAC	-7.12	1.38	1.51
2	B	500	HEM	C2C-C1C	-7.10	1.39	1.52
2	A	500	HEM	C3C-CAC	-7.03	1.38	1.51
2	A	500	HEM	C2C-C1C	-6.73	1.39	1.52
2	D	500	HEM	C2D-C3D	-6.11	1.36	1.54
2	B	500	HEM	C2D-C3D	-6.06	1.36	1.54
2	E	500	HEM	C2D-C3D	-5.96	1.36	1.54
2	C	500	HEM	C2D-C3D	-5.50	1.38	1.54
2	F	500	HEM	C2D-C3D	-5.43	1.38	1.54
2	A	500	HEM	C2D-C3D	-5.11	1.39	1.54
2	B	500	HEM	C3B-CAB	-4.70	1.42	1.51
2	C	500	HEM	C3B-CAB	-4.49	1.42	1.51
2	A	500	HEM	C3B-CAB	-4.48	1.42	1.51
2	C	500	HEM	C1C-NC	-4.35	1.30	1.36
2	D	500	HEM	C3B-CAB	-4.35	1.43	1.51
2	A	500	HEM	C1C-NC	-4.23	1.30	1.36
2	E	500	HEM	C3B-CAB	-4.03	1.43	1.51
2	D	500	HEM	C1C-NC	-3.76	1.31	1.36
2	F	500	HEM	C3B-CAB	-3.55	1.44	1.51
2	E	500	HEM	C2D-C1D	-3.39	1.40	1.51
2	F	500	HEM	C2D-C1D	-3.37	1.40	1.51
2	D	500	HEM	C2D-C1D	-3.29	1.41	1.51
2	B	500	HEM	C2D-C1D	-3.27	1.41	1.51
2	A	500	HEM	C2D-C1D	-3.20	1.41	1.51
2	C	500	HEM	C2D-C1D	-3.08	1.41	1.51
2	B	500	HEM	C2B-C1B	-2.92	1.42	1.51
2	E	500	HEM	C1C-NC	-2.89	1.32	1.36
2	D	500	HEM	C2B-C1B	-2.82	1.42	1.51
2	C	500	HEM	C2B-C1B	-2.79	1.42	1.51
2	A	500	HEM	C2B-C1B	-2.58	1.43	1.51
2	E	500	HEM	C2B-C1B	-2.56	1.43	1.51
2	B	500	HEM	C1C-NC	-2.55	1.32	1.36
2	F	500	HEM	C2B-C1B	-2.40	1.44	1.51
2	F	500	HEM	C1C-NC	-2.30	1.33	1.36
3	E	505[A]	IND	C6-C7	2.01	1.41	1.36
2	B	500	HEM	CMC-C2C	2.06	1.57	1.53
3	F	506[A]	IND	C6-C7	2.06	1.41	1.36
2	E	500	HEM	CMC-C2C	2.07	1.58	1.53
2	D	500	HEM	CMC-C2C	2.08	1.58	1.53
3	D	504[A]	IND	C6-C7	2.10	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	CBC-CAC	2.14	1.41	1.29
2	B	500	HEM	CBC-CAC	2.16	1.41	1.29
3	C	503[A]	IND	C6-C7	2.16	1.41	1.36
2	A	500	HEM	CMA-C3A	2.17	1.56	1.51
3	B	502[A]	IND	C6-C7	2.22	1.41	1.36
2	A	500	HEM	CBC-CAC	2.28	1.42	1.29
2	C	500	HEM	CBC-CAC	2.28	1.42	1.29
2	F	500	HEM	CBC-CAC	2.29	1.42	1.29
2	E	500	HEM	CBC-CAC	2.36	1.42	1.29
2	C	500	HEM	FE-NC	2.72	2.06	1.95
2	B	500	HEM	FE-NC	2.75	2.06	1.95
2	C	500	HEM	CMA-C3A	2.89	1.57	1.51
2	A	500	HEM	CBB-CAB	3.03	1.46	1.29
2	D	500	HEM	FE-NC	3.07	2.07	1.95
2	B	500	HEM	CMA-C3A	3.07	1.58	1.51
2	F	500	HEM	FE-NC	3.11	2.08	1.95
2	D	500	HEM	CMA-C3A	3.12	1.58	1.51
2	D	500	HEM	CBB-CAB	3.22	1.47	1.29
2	B	500	HEM	CBB-CAB	3.22	1.47	1.29
2	E	500	HEM	FE-NC	3.27	2.08	1.95
2	A	500	HEM	FE-NC	3.33	2.08	1.95
2	F	500	HEM	CMA-C3A	3.35	1.58	1.51
2	E	500	HEM	CMA-C3A	3.43	1.58	1.51
2	E	500	HEM	CBB-CAB	3.47	1.49	1.29
2	C	500	HEM	CBB-CAB	3.53	1.49	1.29
2	F	500	HEM	CBB-CAB	3.55	1.49	1.29

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C1D-CHD-C4C	2.15	129.41	125.82
2	D	500	HEM	C1D-CHD-C4C	2.17	129.44	125.82
2	B	500	HEM	C1D-CHD-C4C	2.41	129.85	125.82
2	D	500	HEM	CMD-C2D-C3D	2.51	125.44	114.35
2	C	500	HEM	CMD-C2D-C3D	2.53	125.55	114.35
2	B	500	HEM	CMD-C2D-C3D	2.54	125.60	114.35
2	E	500	HEM	CMD-C2D-C3D	2.58	125.75	114.35
2	F	500	HEM	CMD-C2D-C3D	2.62	125.95	114.35
2	A	500	HEM	CMD-C2D-C3D	2.64	126.03	114.35
2	F	500	HEM	C1D-CHD-C4C	2.68	130.30	125.82
2	E	500	HEM	C1D-CHD-C4C	2.71	130.36	125.82
2	A	500	HEM	C1D-CHD-C4C	2.75	130.42	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	HEM	C3C-CAC-CBC	2.91	128.93	124.46
2	F	500	HEM	C3C-CAC-CBC	3.01	129.07	124.46
2	B	500	HEM	C3C-CAC-CBC	3.14	129.28	124.46
2	B	500	HEM	C4B-CHC-C1C	3.19	131.15	125.82
2	E	500	HEM	C4B-CHC-C1C	3.39	131.48	125.82
2	A	500	HEM	C4B-CHC-C1C	3.50	131.67	125.82
2	A	500	HEM	CAD-C3D-C4D	3.58	125.09	112.47
2	F	500	HEM	C4B-CHC-C1C	3.74	132.07	125.82
2	A	500	HEM	C3C-CAC-CBC	3.81	130.30	124.46
2	D	500	HEM	C3C-CAC-CBC	3.81	130.31	124.46
2	D	500	HEM	CAD-C3D-C4D	3.83	125.96	112.47
2	D	500	HEM	C4B-CHC-C1C	3.86	132.28	125.82
2	B	500	HEM	C3B-CAB-CBB	3.93	130.48	124.46
2	C	500	HEM	C3C-CAC-CBC	4.03	130.64	124.46
2	B	500	HEM	CAD-C3D-C4D	4.04	126.73	112.47
2	A	500	HEM	CMC-C2C-C3C	4.07	126.68	116.53
2	C	500	HEM	C4B-CHC-C1C	4.10	132.68	125.82
2	F	500	HEM	CAD-C3D-C4D	4.12	127.00	112.47
2	E	500	HEM	CAD-C3D-C4D	4.19	127.24	112.47
2	B	500	HEM	CMC-C2C-C3C	4.19	127.00	116.53
2	C	500	HEM	CAD-C3D-C4D	4.27	127.54	112.47
2	E	500	HEM	CMC-C2C-C3C	4.28	127.21	116.53
2	C	500	HEM	CMC-C2C-C3C	4.30	127.27	116.53
2	D	500	HEM	C3B-CAB-CBB	4.33	131.09	124.46
2	F	500	HEM	CMC-C2C-C3C	4.35	127.39	116.53
2	C	500	HEM	C3B-CAB-CBB	4.46	131.30	124.46
2	D	500	HEM	CMC-C2C-C3C	4.67	128.20	116.53
2	F	500	HEM	C3B-CAB-CBB	4.85	131.89	124.46
2	A	500	HEM	C3B-CAB-CBB	4.87	131.93	124.46
2	E	500	HEM	C3B-CAB-CBB	5.07	132.24	124.46
2	E	500	HEM	CAD-C3D-C2D	5.32	128.52	113.22
2	F	500	HEM	CMB-C2B-C3B	5.37	129.92	116.53
2	B	500	HEM	CAD-C3D-C2D	5.39	128.71	113.22
2	F	500	HEM	CAD-C3D-C2D	5.40	128.74	113.22
2	C	500	HEM	CMB-C2B-C3B	5.42	130.06	116.53
2	A	500	HEM	CMB-C2B-C3B	5.43	130.09	116.53
2	C	500	HEM	CAD-C3D-C2D	5.43	128.84	113.22
2	D	500	HEM	CMB-C2B-C3B	5.43	130.09	116.53
2	E	500	HEM	CMB-C2B-C3B	5.52	130.32	116.53
2	D	500	HEM	CAD-C3D-C2D	5.61	129.34	113.22
2	B	500	HEM	CMB-C2B-C3B	5.92	131.29	116.53
2	A	500	HEM	CAD-C3D-C2D	6.10	130.77	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	1	0
3	A	507[B]	IND	1	0
2	B	500	HEM	3	0
3	B	508[B]	IND	5	0
2	C	500	HEM	3	0
3	C	503[A]	IND	1	0
3	C	509[B]	IND	1	0
2	D	500	HEM	4	0
3	E	511[B]	IND	2	0
2	F	500	HEM	5	0
3	F	512[B]	IND	2	0

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	464/476 (97%)	-0.09	13 (2%)	56	69	15, 31, 56, 76	0
1	B	464/476 (97%)	0.37	40 (8%)	13	21	16, 43, 73, 86	0
1	C	464/476 (97%)	0.50	55 (11%)	6	10	19, 49, 79, 90	0
1	D	464/476 (97%)	0.15	27 (5%)	26	40	20, 39, 67, 79	0
1	E	464/476 (97%)	0.20	35 (7%)	17	26	22, 41, 72, 84	0
1	F	464/476 (97%)	0.65	60 (12%)	5	9	19, 52, 79, 91	0
All	All	2784/2856 (97%)	0.30	230 (8%)	14	22	15, 42, 75, 91	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	ARG	5.8
1	C	280	LYS	5.1
1	D	306	VAL	5.0
1	D	301	ALA	5.0
1	D	310	LEU	4.9
1	F	492	LEU	4.8
1	B	421	GLY	4.8
1	F	301	ALA	4.8
1	C	259	LEU	4.6
1	C	194	GLU	4.4
1	D	305	THR	4.4
1	C	422	GLN	4.4
1	E	306	VAL	4.4
1	C	178	VAL	4.4
1	D	422	GLN	4.3
1	B	472	ASP	4.3
1	C	348	LYS	4.3
1	F	453	PHE	4.3
1	C	420	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	468	PRO	4.2
1	F	417	LEU	4.2
1	F	282	PRO	4.2
1	C	491	PHE	4.1
1	C	468	PRO	4.1
1	F	310	LEU	4.0
1	C	282	PRO	4.0
1	F	306	VAL	3.9
1	E	305	THR	3.9
1	C	338	ASN	3.9
1	F	420	LYS	3.9
1	E	307	SER	3.9
1	B	471	ILE	3.8
1	F	305	THR	3.7
1	B	301	ALA	3.7
1	F	178	VAL	3.7
1	E	310	LEU	3.6
1	F	343	PHE	3.6
1	F	335	ILE	3.6
1	D	303	THR	3.5
1	F	303	THR	3.5
1	F	280	LYS	3.5
1	B	470	ASP	3.5
1	F	366	LEU	3.5
1	F	449	LEU	3.5
1	C	469	LYS	3.4
1	C	466	GLN	3.4
1	F	339	ARG	3.4
1	C	419	LYS	3.3
1	F	189	ASP	3.3
1	F	423	PHE	3.3
1	F	403	ARG	3.3
1	E	303	THR	3.3
1	F	300	PHE	3.3
1	B	419	LYS	3.3
1	E	470	ASP	3.3
1	F	338	ASN	3.2
1	D	417	LEU	3.2
1	F	307	SER	3.2
1	B	338	ASN	3.2
1	F	145	ILE	3.2
1	B	417	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	452	PHE	3.2
1	F	331	ILE	3.2
1	F	422	GLN	3.2
1	F	428	ALA	3.2
1	D	307	SER	3.2
1	F	147	GLU	3.2
1	B	420	LYS	3.1
1	D	423	PHE	3.1
1	F	283	ASN	3.1
1	A	310	LEU	3.1
1	D	178	VAL	3.1
1	A	305	THR	3.1
1	B	310	LEU	3.1
1	B	284	THR	3.1
1	C	167	ASN	3.1
1	D	309	THR	3.1
1	C	174	LEU	3.0
1	C	470	ASP	3.0
1	D	466	GLN	3.0
1	D	421	GLY	3.0
1	A	306	VAL	3.0
1	D	465	PRO	3.0
1	C	494	ARG	2.9
1	D	420	LYS	2.9
1	C	168	ILE	2.9
1	C	418	ASP	2.9
1	F	336	GLY	2.9
1	F	404	PHE	2.9
1	C	301	ALA	2.9
1	F	418	ASP	2.9
1	D	302	GLY	2.9
1	B	423	PHE	2.9
1	C	310	LEU	2.9
1	F	174	LEU	2.9
1	B	283	ASN	2.9
1	E	301	ALA	2.8
1	F	371	ALA	2.8
1	C	258	THR	2.8
1	B	280	LYS	2.8
1	C	283	ASN	2.8
1	B	466	GLN	2.8
1	E	467	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	470	ASP	2.7
1	A	338	ASN	2.7
1	C	465	PRO	2.7
1	F	407	ASN	2.7
1	B	143	ARG	2.7
1	E	469	LYS	2.7
1	A	262	ASN	2.7
1	C	423	PHE	2.7
1	A	263	SER	2.7
1	B	194	GLU	2.7
1	B	449	LEU	2.7
1	D	300	PHE	2.7
1	F	419	LYS	2.7
1	B	276	GLN	2.7
1	B	279	GLU	2.7
1	C	493	PRO	2.7
1	C	239	LYS	2.7
1	E	347	ALA	2.6
1	F	445	ALA	2.6
1	E	418	ASP	2.6
1	E	417	LEU	2.6
1	E	302	GLY	2.6
1	C	452	PHE	2.6
1	C	453	PHE	2.6
1	B	407	ASN	2.6
1	A	301	ALA	2.6
1	F	298	LEU	2.6
1	C	182	ILE	2.6
1	C	456	ILE	2.6
1	F	416	PHE	2.6
1	E	280	LYS	2.6
1	E	309	THR	2.6
1	D	453	PHE	2.6
1	C	449	LEU	2.6
1	C	166	ALA	2.6
1	D	449	LEU	2.6
1	E	337	LYS	2.6
1	B	282	PRO	2.5
1	E	334	VAL	2.5
1	F	456	ILE	2.5
1	D	338	ASN	2.5
1	C	492	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	308	THR	2.5
1	A	257	ARG	2.5
1	F	370	LEU	2.5
1	C	175	SER	2.5
1	E	323	VAL	2.5
1	C	281	ASN	2.5
1	C	256	GLN	2.5
1	F	143	ARG	2.5
1	C	303	THR	2.5
1	D	283	ASN	2.4
1	A	365	MET	2.4
1	F	409	ARG	2.4
1	F	452	PHE	2.4
1	B	467	SER	2.4
1	C	332	ASP	2.4
1	F	299	PHE	2.4
1	F	194	GLU	2.4
1	F	348	LYS	2.4
1	C	309	THR	2.4
1	B	337	LYS	2.4
1	E	449	LEU	2.4
1	C	421	GLY	2.4
1	E	163	THR	2.4
1	C	459	ASN	2.3
1	E	338	ASN	2.3
1	F	297	ASN	2.3
1	D	308	THR	2.3
1	A	449	LEU	2.3
1	F	196	LYS	2.3
1	B	422	GLN	2.3
1	B	418	ASP	2.3
1	C	192	ASP	2.3
1	B	138	PHE	2.3
1	E	300	PHE	2.3
1	C	307	SER	2.3
1	B	356	ILE	2.3
1	A	308	THR	2.3
1	B	31	GLY	2.3
1	B	303	THR	2.3
1	B	336	GLY	2.3
1	E	143	ARG	2.3
1	A	309	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	445	ALA	2.2
1	F	427	ASP	2.2
1	F	122	GLU	2.2
1	F	84	HIS	2.2
1	B	453	PHE	2.2
1	C	416	PHE	2.2
1	E	174	LEU	2.2
1	C	488	THR	2.2
1	B	300	PHE	2.2
1	E	439	CYS	2.2
1	A	445	ALA	2.2
1	D	168	ILE	2.2
1	B	465	PRO	2.2
1	F	67	PRO	2.2
1	C	279	GLU	2.2
1	F	80	VAL	2.2
1	D	366	LEU	2.2
1	B	263	SER	2.1
1	C	305	THR	2.1
1	D	280	LYS	2.1
1	D	491	PHE	2.1
1	D	163	THR	2.1
1	C	276	GLN	2.1
1	E	194	GLU	2.1
1	C	341	PRO	2.1
1	E	420	LYS	2.1
1	B	329	GLU	2.1
1	E	465	PRO	2.1
1	E	308	THR	2.1
1	F	392	PHE	2.1
1	B	445	ALA	2.1
1	B	182	ILE	2.1
1	E	32	LYS	2.1
1	C	344	GLU	2.0
1	C	141	GLY	2.0
1	F	66	GLY	2.0
1	F	391	VAL	2.0
1	E	419	LYS	2.0
1	F	462	PHE	2.0
1	B	281	ASN	2.0
1	E	173	PHE	2.0
1	E	423	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	339	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	IND	A	507[B]	9/9	0.89	0.45	4.85	31,31,31,31	9
3	IND	C	509[B]	9/9	0.95	0.38	4.20	31,31,31,31	9
3	IND	E	511[B]	9/9	0.83	0.43	3.42	31,31,31,31	9
3	IND	E	505[A]	9/9	0.90	0.36	3.06	31,31,31,31	9
3	IND	A	501[A]	9/9	0.89	0.36	2.89	31,31,31,31	9
3	IND	C	503[A]	9/9	0.95	0.29	2.08	31,31,31,31	9
3	IND	D	504[A]	9/9	0.93	0.36	2.04	31,31,31,31	9
3	IND	D	510[B]	9/9	0.92	0.39	1.78	31,31,31,31	9
3	IND	B	502[A]	9/9	0.95	0.25	1.01	31,31,31,31	9
3	IND	B	508[B]	9/9	0.95	0.24	0.80	31,31,31,31	9
3	IND	F	506[A]	9/9	0.91	0.30	0.65	31,31,31,31	9
3	IND	F	512[B]	9/9	0.92	0.29	0.62	31,31,31,31	9
2	HEM	E	500	43/43	0.97	0.21	0.30	26,34,39,41	0
2	HEM	A	500	43/43	0.98	0.20	0.25	14,20,28,38	0
2	HEM	C	500	43/43	0.96	0.17	-0.03	12,30,41,45	0
2	HEM	F	500	43/43	0.95	0.20	-0.10	23,41,54,61	0
2	HEM	D	500	43/43	0.97	0.17	-0.18	18,27,33,35	0
2	HEM	B	500	43/43	0.98	0.16	-0.19	9,22,34,41	0

6.5 Other polymers

There are no such residues in this entry.