



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:23 am GMT

PDB ID : 2F9Q
Title : Crystal Structure of Human Cytochrome P450 2D6
Authors : Rowland, P.
Deposited on : 2005-12-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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 : trunk28620
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) : recalc28949

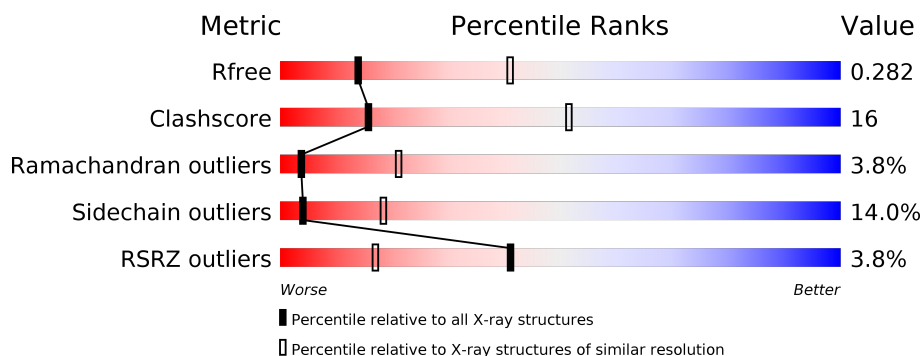
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	479	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	479	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	479	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	479	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>6%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	2000	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14421 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 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3569	2281	634	639	15			
1	B	451	Total	C	N	O	S	0	0	0
			3545	2265	630	635	15			
1	C	454	Total	C	N	O	S	0	0	0
			3569	2281	634	639	15			
1	D	451	Total	C	N	O	S	0	0	0
			3545	2265	630	635	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	HIS	CLONING ARTIFACT	UNP P10635
A	25	LYS	ARG	CLONING ARTIFACT	UNP P10635
A	26	LYS	ARG	CLONING ARTIFACT	UNP P10635
A	27	THR	GLN	CLONING ARTIFACT	UNP P10635
A	28	SER	ARG	CLONING ARTIFACT	UNP P10635
A	29	SER	TRP	CLONING ARTIFACT	UNP P10635
A	30	LYS	ALA	CLONING ARTIFACT	UNP P10635
A	31	GLY	ALA	CLONING ARTIFACT	UNP P10635
A	32	LYS	ARG	CLONING ARTIFACT	UNP P10635
A	33	LEU	TYR	CLONING ARTIFACT	UNP P10635
A	230	ASP	LEU	ENGINEERED	UNP P10635
A	231	ARG	LEU	ENGINEERED	UNP P10635
A	498	HIS	-	EXPRESSION TAG	UNP P10635
A	499	HIS	-	EXPRESSION TAG	UNP P10635
A	500	HIS	-	EXPRESSION TAG	UNP P10635
A	501	HIS	-	EXPRESSION TAG	UNP P10635
B	24	ALA	HIS	CLONING ARTIFACT	UNP P10635
B	25	LYS	ARG	CLONING ARTIFACT	UNP P10635
B	26	LYS	ARG	CLONING ARTIFACT	UNP P10635
B	27	THR	GLN	CLONING ARTIFACT	UNP P10635
B	28	SER	ARG	CLONING ARTIFACT	UNP P10635

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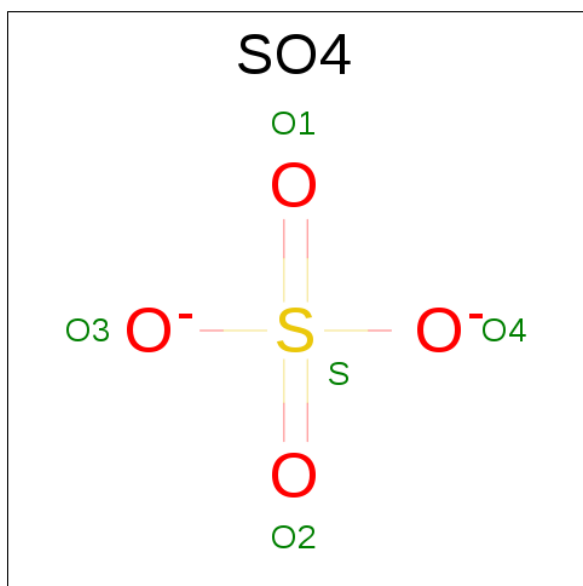
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	TRP	CLONING ARTIFACT	UNP P10635
B	30	LYS	ALA	CLONING ARTIFACT	UNP P10635
B	31	GLY	ALA	CLONING ARTIFACT	UNP P10635
B	32	LYS	ARG	CLONING ARTIFACT	UNP P10635
B	33	LEU	TYR	CLONING ARTIFACT	UNP P10635
B	230	ASP	LEU	ENGINEERED	UNP P10635
B	231	ARG	LEU	ENGINEERED	UNP P10635
B	498	HIS	-	EXPRESSION TAG	UNP P10635
B	499	HIS	-	EXPRESSION TAG	UNP P10635
B	500	HIS	-	EXPRESSION TAG	UNP P10635
B	501	HIS	-	EXPRESSION TAG	UNP P10635
C	24	ALA	HIS	CLONING ARTIFACT	UNP P10635
C	25	LYS	ARG	CLONING ARTIFACT	UNP P10635
C	26	LYS	ARG	CLONING ARTIFACT	UNP P10635
C	27	THR	GLN	CLONING ARTIFACT	UNP P10635
C	28	SER	ARG	CLONING ARTIFACT	UNP P10635
C	29	SER	TRP	CLONING ARTIFACT	UNP P10635
C	30	LYS	ALA	CLONING ARTIFACT	UNP P10635
C	31	GLY	ALA	CLONING ARTIFACT	UNP P10635
C	32	LYS	ARG	CLONING ARTIFACT	UNP P10635
C	33	LEU	TYR	CLONING ARTIFACT	UNP P10635
C	230	ASP	LEU	ENGINEERED	UNP P10635
C	231	ARG	LEU	ENGINEERED	UNP P10635
C	498	HIS	-	EXPRESSION TAG	UNP P10635
C	499	HIS	-	EXPRESSION TAG	UNP P10635
C	500	HIS	-	EXPRESSION TAG	UNP P10635
C	501	HIS	-	EXPRESSION TAG	UNP P10635
D	24	ALA	HIS	CLONING ARTIFACT	UNP P10635
D	25	LYS	ARG	CLONING ARTIFACT	UNP P10635
D	26	LYS	ARG	CLONING ARTIFACT	UNP P10635
D	27	THR	GLN	CLONING ARTIFACT	UNP P10635
D	28	SER	ARG	CLONING ARTIFACT	UNP P10635
D	29	SER	TRP	CLONING ARTIFACT	UNP P10635
D	30	LYS	ALA	CLONING ARTIFACT	UNP P10635
D	31	GLY	ALA	CLONING ARTIFACT	UNP P10635
D	32	LYS	ARG	CLONING ARTIFACT	UNP P10635
D	33	LEU	TYR	CLONING ARTIFACT	UNP P10635
D	230	ASP	LEU	ENGINEERED	UNP P10635
D	231	ARG	LEU	ENGINEERED	UNP P10635
D	498	HIS	-	EXPRESSION TAG	UNP P10635
D	499	HIS	-	EXPRESSION TAG	UNP P10635
D	500	HIS	-	EXPRESSION TAG	UNP P10635

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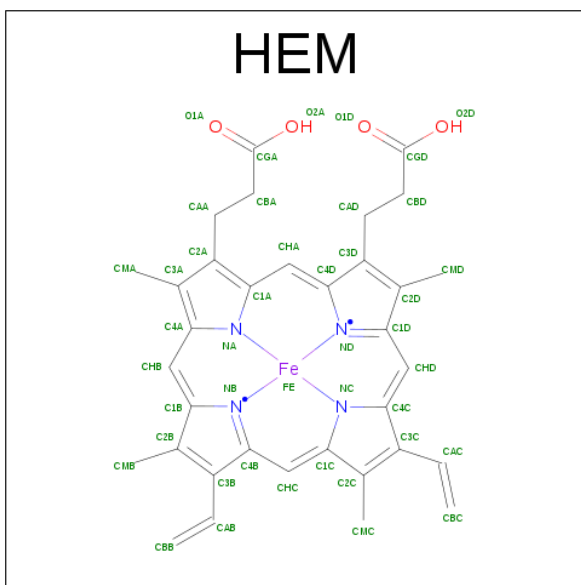
Chain	Residue	Modelled	Actual	Comment	Reference
D	501	HIS	-	EXPRESSION TAG	UNP P10635

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

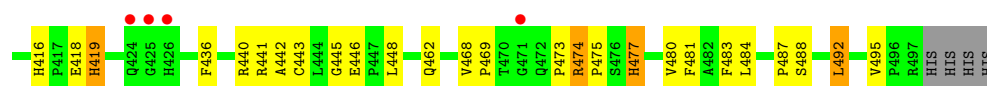
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



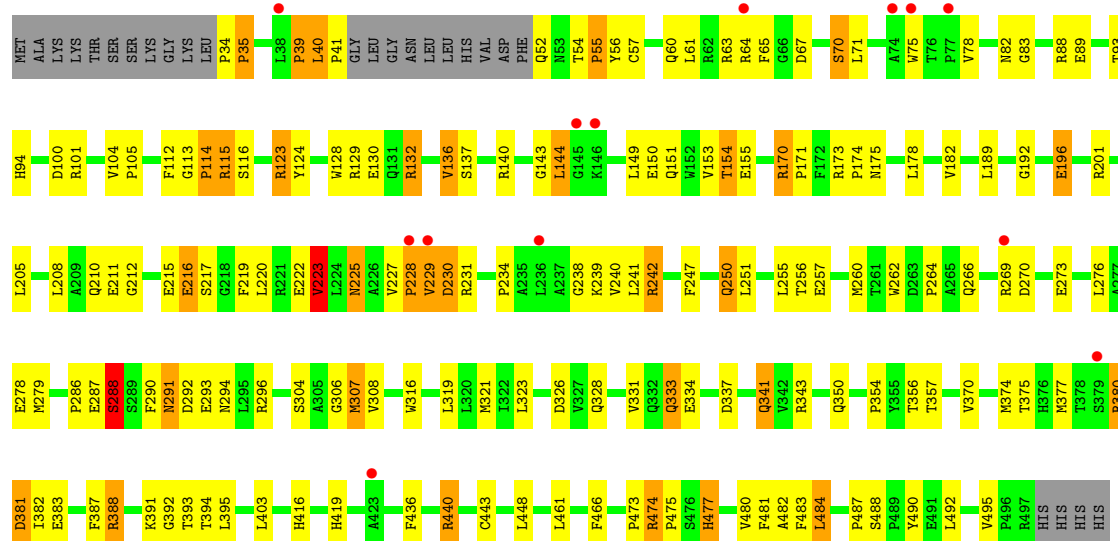
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is water.

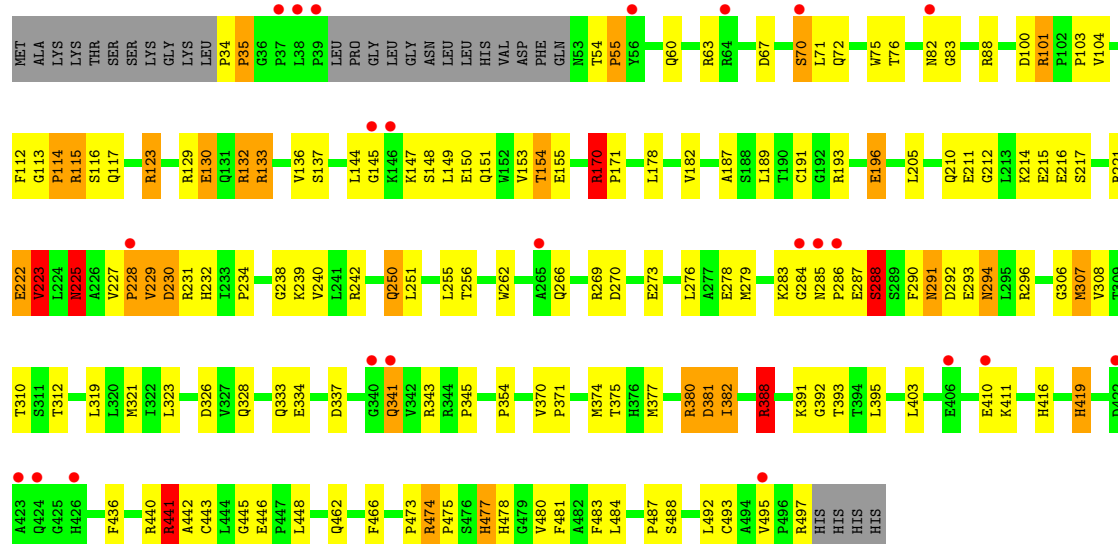
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	3	Total O 3 3	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0



• Molecule 1: Cytochrome P450 2D6



• Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.07Å 155.50Å 95.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.00 – 3.00 39.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (106.00-3.00) 89.6 (39.97-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.230 , 0.286 0.230 , 0.282	Depositor DCC
R_{free} test set	1601 reflections (4.23%)	DCC
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.6	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	0.92	EDS
Total number of atoms	14421	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.79	0/3664	0.82	1/4982 (0.0%)
1	B	0.72	1/3639 (0.0%)	0.80	3/4947 (0.1%)
1	C	0.79	1/3664 (0.0%)	0.84	1/4982 (0.0%)
1	D	0.77	2/3639 (0.1%)	0.82	6/4947 (0.1%)
All	All	0.77	4/14606 (0.0%)	0.82	11/19858 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	ARG	CZ-NH1	15.49	1.53	1.33
1	C	57	CYS	CB-SG	-5.78	1.72	1.81
1	D	269	ARG	CZ-NH2	5.50	1.40	1.33
1	B	161	CYS	CB-SG	-5.42	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	ARG	NE-CZ-NH2	-13.90	113.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	441	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	D	388	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	234	PRO	N-CA-CB	6.54	111.15	103.30
1	B	234	PRO	N-CA-CB	6.44	111.03	103.30
1	C	234	PRO	N-CA-CB	6.30	110.86	103.30
1	A	234	PRO	N-CA-CB	6.04	110.55	103.30
1	D	269	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	492	LEU	CA-CB-CG	5.21	127.27	115.30
1	D	170	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLY	Peptide
1	A	40	LEU	Peptide
1	A	53	ASN	Peptide
1	A	83	GLY	Peptide
1	B	113	GLY	Peptide
1	C	113	GLY	Peptide
1	C	83	GLY	Peptide
1	D	113	GLY	Peptide
1	D	83	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3569	0	3513	126	0
1	B	3545	0	3487	116	0
1	C	3569	0	3513	139	0
1	D	3545	0	3487	125	0
2	B	10	0	0	2	0
3	A	43	0	30	5	0
3	B	43	0	30	6	0
3	C	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	30	8	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	14421	0	14120	468	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 (468) 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:227:VAL:HB	1:C:227:VAL:CB	1.75	1.16
1:B:227:VAL:CB	1:C:227:VAL:HB	1.75	1.15
1:A:60:GLN:NE2	1:B:60:GLN:HE21	1.49	1.11
1:C:60:GLN:HE21	1:D:60:GLN:NE2	1.53	1.05
1:A:60:GLN:NE2	1:B:60:GLN:NE2	2.06	1.03
1:A:60:GLN:HE21	1:B:60:GLN:NE2	1.58	1.00
1:A:287:GLU:O	1:A:288:SER:HB3	1.60	0.98
1:C:287:GLU:O	1:C:288:SER:HB3	1.61	0.97
1:C:40:LEU:H	1:C:41:PRO:HD3	1.29	0.97
1:C:115:ARG:NH2	1:C:286:PRO:O	2.01	0.94
1:A:229:VAL:HA	1:D:75:TRP:O	1.69	0.93
3:D:600:HEM:HBC2	3:D:600:HEM:HMC2	1.50	0.91
1:B:287:GLU:O	1:B:288:SER:HB3	1.70	0.90
1:A:227:VAL:CG2	1:A:228:PRO:HD2	2.03	0.89
1:D:227:VAL:CG2	1:D:228:PRO:HD2	2.04	0.88
1:D:34:PRO:HD3	1:D:388:ARG:NH1	1.90	0.87
1:A:227:VAL:HG13	1:D:76:THR:HG23	1.56	0.87
1:B:227:VAL:CG2	1:B:228:PRO:HD2	2.04	0.86
1:D:287:GLU:O	1:D:288:SER:HB3	1.74	0.85
1:C:227:VAL:CG2	1:C:228:PRO:HD2	2.06	0.85
1:A:227:VAL:CG1	1:D:76:THR:HG23	2.07	0.84
1:A:60:GLN:HE21	1:B:60:GLN:HE21	0.85	0.84
1:C:473:PRO:O	1:C:474:ARG:HB3	1.78	0.84
1:A:227:VAL:HG23	1:A:228:PRO:HD2	1.60	0.84
1:C:227:VAL:HG23	1:C:228:PRO:HD2	1.59	0.82
1:B:227:VAL:HG23	1:B:228:PRO:HD2	1.59	0.82
1:C:39:PRO:HB2	1:C:41:PRO:HD3	1.62	0.81
1:D:211:GLU:O	1:D:215:GLU:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PRO:HD3	1:C:388:ARG:NH1	1.97	0.80
1:C:40:LEU:H	1:C:41:PRO:CD	1.94	0.80
1:A:76:THR:HG23	1:D:227:VAL:CG1	2.12	0.80
1:D:473:PRO:O	1:D:474:ARG:HB3	1.81	0.80
1:D:227:VAL:HG23	1:D:228:PRO:HD2	1.62	0.79
1:A:39:PRO:HB2	1:A:41:PRO:HD3	1.63	0.79
1:A:76:THR:HG23	1:D:227:VAL:HG13	1.66	0.78
3:D:600:HEM:HBC2	3:D:600:HEM:CMC	2.13	0.78
1:A:34:PRO:HD3	1:A:388:ARG:NH1	2.00	0.77
1:B:221:ARG:NH2	1:C:41:PRO:O	2.18	0.77
1:C:137:SER:HA	1:C:140:ARG:NH2	2.00	0.76
1:A:75:TRP:O	1:D:229:VAL:HA	1.86	0.75
1:B:211:GLU:O	1:B:215:GLU:HG3	1.86	0.75
3:B:600:HEM:HBC2	3:B:600:HEM:HMC2	1.68	0.74
3:B:600:HEM:CMC	3:B:600:HEM:HBC2	2.18	0.74
1:B:34:PRO:HD3	1:B:388:ARG:NH1	2.02	0.74
1:C:211:GLU:O	1:C:215:GLU:HG3	1.85	0.74
1:A:473:PRO:O	1:A:474:ARG:HB3	1.86	0.73
1:B:321:MET:CE	1:B:328:GLN:HA	2.17	0.73
1:D:229:VAL:O	1:D:231:ARG:N	2.17	0.73
1:B:473:PRO:O	1:B:474:ARG:HB3	1.90	0.72
1:C:40:LEU:N	1:C:41:PRO:HD3	2.04	0.71
1:B:129:ARG:NH1	2:B:2000:SO4:O3	2.23	0.71
1:D:196:GLU:HA	1:D:196:GLU:OE2	1.88	0.71
1:C:56:TYR:O	1:D:60:GLN:NE2	2.24	0.71
1:B:133:ARG:NH2	2:B:2000:SO4:O2	2.23	0.71
1:A:278:GLU:HG2	1:A:290:PHE:CZ	2.25	0.71
1:C:115:ARG:HE	1:C:287:GLU:HA	1.55	0.71
3:A:600:HEM:HBC2	3:A:600:HEM:HMC2	1.73	0.71
1:A:306:GLY:HA2	3:A:600:HEM:C2C	2.25	0.70
1:C:321:MET:HE1	1:C:328:GLN:HA	1.74	0.70
1:D:133:ARG:HH11	1:D:133:ARG:HG2	1.57	0.70
1:D:388:ARG:HG2	1:D:388:ARG:HH11	1.55	0.70
1:A:388:ARG:HG2	1:A:388:ARG:HH11	1.57	0.70
3:C:600:HEM:HMC2	3:C:600:HEM:HBC2	1.73	0.70
1:A:211:GLU:O	1:A:215:GLU:HG3	1.91	0.69
1:B:278:GLU:HG2	1:B:290:PHE:CZ	2.27	0.69
1:D:117:GLN:O	1:D:294:ASN:ND2	2.20	0.69
1:C:278:GLU:HG2	1:C:290:PHE:CZ	2.28	0.69
1:B:388:ARG:HG2	1:B:388:ARG:HH11	1.57	0.68
1:D:34:PRO:HD3	1:D:388:ARG:HH12	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:O	1:A:155:GLU:HG2	1.92	0.68
1:D:321:MET:CE	1:D:328:GLN:HA	2.23	0.68
1:C:229:VAL:O	1:C:231:ARG:N	2.21	0.68
1:A:196:GLU:HA	1:A:196:GLU:OE2	1.93	0.68
1:A:227:VAL:CG1	1:D:76:THR:CG2	2.72	0.68
1:C:143:GLY:C	1:C:144:LEU:HG	2.14	0.67
1:C:388:ARG:HG2	1:C:388:ARG:HH11	1.58	0.67
1:D:104:VAL:HG12	1:D:223:VAL:HG21	1.77	0.67
1:A:56:TYR:HB3	1:B:60:GLN:HG3	1.76	0.66
1:C:151:GLN:O	1:C:155:GLU:HG2	1.95	0.66
1:C:205:LEU:HD12	1:C:250:GLN:NE2	2.10	0.66
1:A:54:THR:H	1:A:55:PRO:HD3	1.61	0.66
1:A:76:THR:CG2	1:D:227:VAL:HG11	2.25	0.66
1:D:381:ASP:O	1:D:382:ILE:HD13	1.96	0.66
1:B:306:GLY:HA2	3:B:600:HEM:C2C	2.29	0.66
1:D:217:SER:O	1:D:221:ARG:HG2	1.94	0.66
1:B:170:ARG:HD2	1:B:171:PRO:HD2	1.76	0.66
1:C:321:MET:CE	1:C:328:GLN:HA	2.26	0.65
1:D:34:PRO:CD	1:D:388:ARG:HH12	2.09	0.65
1:B:104:VAL:HG12	1:B:223:VAL:HG21	1.78	0.65
1:A:227:VAL:HG11	1:D:76:THR:CG2	2.26	0.65
1:B:205:LEU:HD12	1:B:250:GLN:NE2	2.12	0.65
1:C:39:PRO:CB	1:C:41:PRO:HD3	2.27	0.64
1:C:34:PRO:HD3	1:C:388:ARG:HH12	1.59	0.64
1:C:64:ARG:CZ	1:D:478:HIS:CE1	2.81	0.64
1:B:178:LEU:O	1:B:182:VAL:HG23	1.98	0.64
1:A:34:PRO:HD3	1:A:388:ARG:HH12	1.61	0.64
1:B:96:GLU:HG3	1:B:124:TYR:OH	1.98	0.64
1:B:321:MET:HE1	1:B:328:GLN:HA	1.79	0.63
1:C:229:VAL:C	1:C:231:ARG:H	2.02	0.63
1:D:278:GLU:HG2	1:D:290:PHE:CZ	2.35	0.62
1:A:76:THR:CG2	1:D:227:VAL:CG1	2.77	0.62
1:A:436:PHE:HB3	1:A:443:CYS:HB3	1.80	0.62
1:D:306:GLY:HA2	3:D:600:HEM:C2C	2.33	0.62
1:A:229:VAL:O	1:A:231:ARG:N	2.25	0.62
1:C:477:HIS:H	1:C:477:HIS:CD2	2.16	0.62
1:D:149:LEU:O	1:D:153:VAL:HG23	2.00	0.62
1:B:114:PRO:HB2	1:B:115:ARG:CZ	2.30	0.62
1:A:229:VAL:C	1:A:231:ARG:H	2.03	0.62
1:B:278:GLU:OE1	1:B:281:LYS:NZ	2.24	0.62
1:A:222:GLU:HB3	1:D:75:TRP:CZ2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PRO:HD3	1:B:388:ARG:HH12	1.65	0.61
1:D:477:HIS:H	1:D:477:HIS:CD2	2.16	0.61
1:A:104:VAL:HG12	1:A:223:VAL:HG21	1.81	0.61
1:B:227:VAL:CG2	1:B:228:PRO:CD	2.76	0.61
1:C:377:MET:HA	1:C:393:THR:O	2.00	0.61
1:C:306:GLY:HA2	3:C:600:HEM:C2C	2.35	0.61
1:A:60:GLN:HG3	1:B:56:TYR:HB3	1.82	0.61
1:C:64:ARG:HH22	1:D:478:HIS:CG	2.19	0.61
1:C:60:GLN:NE2	1:D:60:GLN:NE2	2.38	0.61
1:C:104:VAL:HG12	1:C:223:VAL:HG21	1.83	0.61
1:C:60:GLN:HE21	1:D:60:GLN:HE21	1.47	0.61
1:C:64:ARG:NH2	1:D:478:HIS:CG	2.69	0.61
1:A:189:LEU:O	1:A:270:ASP:HB2	2.01	0.60
3:A:600:HEM:CMC	3:A:600:HEM:HBC2	2.31	0.60
1:B:279:MET:HG3	1:B:290:PHE:O	2.02	0.60
1:C:223:VAL:O	1:C:223:VAL:HG13	2.02	0.59
1:A:321:MET:CE	1:A:328:GLN:HA	2.33	0.59
1:C:227:VAL:CG2	1:C:228:PRO:CD	2.79	0.59
1:C:39:PRO:HB2	1:C:41:PRO:CD	2.32	0.59
1:C:149:LEU:O	1:C:153:VAL:HG23	2.02	0.59
1:D:321:MET:HE3	1:D:328:GLN:HA	1.84	0.58
1:D:34:PRO:CD	1:D:388:ARG:NH1	2.64	0.58
1:A:192:GLY:CA	1:A:269:ARG:HH22	2.17	0.57
1:D:205:LEU:HD12	1:D:250:GLN:NE2	2.18	0.57
1:B:227:VAL:HG22	1:B:228:PRO:CD	2.34	0.57
1:C:380:ARG:HA	1:C:391:LYS:HG3	1.86	0.57
1:B:208:LEU:HB3	1:B:247:PHE:HB2	1.86	0.57
1:A:205:LEU:HD12	1:A:250:GLN:NE2	2.20	0.57
1:B:132:ARG:O	1:B:136:VAL:HG13	2.05	0.57
3:C:600:HEM:HBC2	3:C:600:HEM:CMC	2.35	0.57
1:D:380:ARG:HG2	1:D:380:ARG:HH11	1.71	0.56
1:A:276:LEU:HA	1:A:279:MET:HE3	1.87	0.56
1:A:223:VAL:HG13	1:A:223:VAL:O	2.04	0.56
1:C:436:PHE:HB3	1:C:443:CYS:HB3	1.87	0.56
1:C:178:LEU:O	1:C:182:VAL:HG23	2.05	0.56
1:D:279:MET:HG3	1:D:290:PHE:O	2.06	0.56
1:B:436:PHE:HB3	1:B:443:CYS:HB3	1.88	0.56
1:A:374:MET:SD	1:A:375:THR:HG22	2.45	0.56
1:A:443:CYS:HB2	3:A:600:HEM:NA	2.21	0.56
1:A:238:GLY:O	1:A:240:VAL:N	2.39	0.56
1:C:60:GLN:HE21	1:D:60:GLN:HE22	1.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:HIS:CD2	1:B:477:HIS:H	2.23	0.55
1:B:151:GLN:O	1:B:155:GLU:HG2	2.07	0.55
1:C:64:ARG:NH1	1:D:478:HIS:ND1	2.55	0.55
1:B:229:VAL:C	1:B:231:ARG:H	2.10	0.55
1:B:276:LEU:HA	1:B:279:MET:HE3	1.89	0.55
1:C:276:LEU:HA	1:C:279:MET:HE3	1.89	0.55
1:A:477:HIS:H	1:A:477:HIS:CD2	2.24	0.55
1:C:196:GLU:HA	1:C:196:GLU:OE2	2.07	0.55
1:A:103:PRO:HD3	1:A:123:ARG:HH21	1.70	0.54
1:B:377:MET:HA	1:B:393:THR:O	2.07	0.54
1:C:227:VAL:HG22	1:C:228:PRO:CD	2.37	0.54
1:C:443:CYS:HB2	3:C:600:HEM:NA	2.21	0.54
1:A:377:MET:HA	1:A:393:THR:O	2.07	0.54
1:B:229:VAL:O	1:B:231:ARG:N	2.28	0.54
1:B:321:MET:HE3	1:B:328:GLN:HA	1.89	0.54
1:A:170:ARG:HD2	1:A:171:PRO:HD2	1.89	0.54
1:C:251:LEU:O	1:C:255:LEU:HG	2.07	0.54
1:D:223:VAL:HG13	1:D:223:VAL:O	2.08	0.54
1:B:103:PRO:HD3	1:B:123:ARG:HH21	1.72	0.54
1:D:251:LEU:O	1:D:255:LEU:HG	2.08	0.54
1:B:381:ASP:O	1:B:382:ILE:HD13	2.07	0.53
1:C:170:ARG:HD2	1:C:171:PRO:HD2	1.90	0.53
1:D:227:VAL:HG22	1:D:228:PRO:HD2	1.88	0.53
1:A:227:VAL:HG22	1:A:228:PRO:HD2	1.88	0.53
1:B:196:GLU:OE2	1:B:196:GLU:HA	2.07	0.53
1:D:212:GLY:O	1:D:216:GLU:HG2	2.07	0.53
1:B:212:GLY:O	1:B:216:GLU:HG2	2.09	0.53
1:D:132:ARG:NH1	1:D:441:ARG:HA	2.23	0.53
1:C:212:GLY:O	1:C:216:GLU:HG2	2.08	0.53
1:D:377:MET:HA	1:D:393:THR:O	2.08	0.53
1:D:133:ARG:NH1	1:D:133:ARG:HG2	2.24	0.53
1:C:56:TYR:HB3	1:D:60:GLN:CD	2.29	0.53
1:B:149:LEU:O	1:B:153:VAL:HG23	2.08	0.53
1:B:381:ASP:OD2	1:B:381:ASP:N	2.41	0.53
1:D:170:ARG:HD2	1:D:171:PRO:HD2	1.90	0.53
1:A:279:MET:HG3	1:A:290:PHE:O	2.10	0.52
1:B:35:PRO:O	1:B:70:SER:HB2	2.09	0.52
1:D:319:LEU:HD22	1:D:487:PRO:HB3	1.91	0.52
1:A:462:GLN:O	1:A:497:ARG:NH1	2.42	0.52
1:C:381:ASP:O	1:C:382:ILE:HD13	2.08	0.52
1:D:436:PHE:HB3	1:D:443:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:O	1:B:223:VAL:HG13	2.09	0.52
1:A:321:MET:HE1	1:A:328:GLN:HA	1.90	0.52
1:A:383:GLU:HA	1:A:387:PHE:O	2.09	0.52
1:D:388:ARG:HG2	1:D:388:ARG:NH1	2.24	0.52
1:A:40:LEU:N	1:A:41:PRO:HD3	2.25	0.52
1:D:114:PRO:HB2	1:D:115:ARG:HG2	1.90	0.52
1:D:151:GLN:O	1:D:155:GLU:HG2	2.10	0.52
1:D:170:ARG:CD	1:D:171:PRO:HD2	2.40	0.52
1:D:229:VAL:C	1:D:231:ARG:H	2.09	0.51
1:A:380:ARG:HA	1:A:391:LYS:HG3	1.92	0.51
1:A:381:ASP:O	1:A:382:ILE:HD13	2.10	0.51
3:D:600:HEM:HBB2	3:D:600:HEM:CMB	2.41	0.51
1:D:481:PHE:CG	1:D:481:PHE:O	2.62	0.51
1:A:178:LEU:O	1:A:182:VAL:HG23	2.10	0.51
1:D:443:CYS:HB2	3:D:600:HEM:NA	2.26	0.51
1:A:227:VAL:HG22	1:A:228:PRO:CD	2.39	0.51
1:C:64:ARG:NH2	1:D:478:HIS:CD2	2.78	0.51
1:D:321:MET:HE1	1:D:328:GLN:HA	1.90	0.51
1:A:227:VAL:HG11	1:D:76:THR:HG21	1.92	0.51
1:D:129:ARG:O	1:D:133:ARG:HB2	2.10	0.51
1:D:35:PRO:O	1:D:70:SER:HB2	2.10	0.51
1:C:64:ARG:CZ	1:D:478:HIS:ND1	2.73	0.50
1:D:345:PRO:HD3	1:D:462:GLN:HE22	1.77	0.50
1:A:319:LEU:HD22	1:A:487:PRO:HB3	1.93	0.50
1:A:341:GLN:HE21	1:A:341:GLN:HA	1.77	0.50
1:B:227:VAL:CG2	1:C:227:VAL:CG2	2.89	0.50
1:A:307:MET:HG2	1:A:308:VAL:N	2.27	0.50
1:D:308:VAL:O	1:D:312:THR:OG1	2.27	0.50
1:A:388:ARG:HG2	1:A:388:ARG:NH1	2.25	0.50
1:D:307:MET:HG2	1:D:308:VAL:N	2.25	0.50
1:A:34:PRO:CD	1:A:388:ARG:HH12	2.25	0.50
1:D:238:GLY:O	1:D:240:VAL:N	2.45	0.50
1:A:227:VAL:CG2	1:A:228:PRO:CD	2.82	0.50
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.47	0.49
1:C:35:PRO:O	1:C:70:SER:HB2	2.12	0.49
1:D:189:LEU:O	1:D:270:ASP:HB2	2.11	0.49
1:D:276:LEU:HA	1:D:279:MET:HE3	1.92	0.49
1:A:208:LEU:HB3	1:A:247:PHE:HB2	1.94	0.49
1:C:341:GLN:HE21	1:C:341:GLN:HA	1.77	0.49
1:C:388:ARG:HG2	1:C:388:ARG:NH1	2.26	0.49
1:B:374:MET:SD	1:B:375:THR:HG22	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LEU:O	1:C:270:ASP:HB2	2.13	0.49
1:C:279:MET:HG3	1:C:290:PHE:O	2.13	0.49
1:D:381:ASP:OD2	1:D:381:ASP:N	2.46	0.49
1:A:40:LEU:H	1:A:41:PRO:CD	2.25	0.49
1:B:253:GLU:HG2	1:B:254:LEU:N	2.27	0.49
1:C:333:GLN:NE2	1:C:333:GLN:HA	2.28	0.49
1:D:227:VAL:HG22	1:D:228:PRO:CD	2.42	0.49
1:C:114:PRO:HB2	1:C:115:ARG:HD3	1.94	0.49
1:B:319:LEU:HD22	1:B:487:PRO:HB3	1.94	0.48
1:D:149:LEU:HD13	1:D:448:LEU:HD13	1.94	0.48
1:C:56:TYR:HB3	1:D:60:GLN:CG	2.43	0.48
1:A:371:PRO:HG2	1:A:481:PHE:HE1	1.78	0.48
1:A:76:THR:HG21	1:D:227:VAL:HG11	1.95	0.48
1:C:334:GLU:OE1	1:C:354:PRO:HD2	2.13	0.48
1:C:56:TYR:HB3	1:D:60:GLN:HG3	1.95	0.48
1:C:137:SER:HA	1:C:140:ARG:HH21	1.77	0.48
1:C:383:GLU:HA	1:C:387:PHE:O	2.12	0.48
1:C:78:VAL:HG22	1:C:394:THR:HB	1.94	0.48
1:D:334:GLU:OE1	1:D:354:PRO:HD2	2.14	0.48
1:B:319:LEU:O	1:B:323:LEU:HB2	2.13	0.48
1:B:208:LEU:HD22	1:B:246:ALA:HB3	1.96	0.48
1:B:94:HIS:ND1	1:B:382:ILE:HD12	2.29	0.48
1:C:374:MET:SD	1:C:375:THR:HG22	2.53	0.48
1:C:481:PHE:O	1:C:481:PHE:CG	2.64	0.48
1:A:333:GLN:HA	1:A:333:GLN:NE2	2.28	0.48
1:B:443:CYS:HB2	3:B:600:HEM:NA	2.28	0.48
1:C:192:GLY:HA2	1:C:269:ARG:HH12	1.79	0.48
1:D:55:PRO:HD3	1:D:481:PHE:CE2	2.49	0.48
1:A:319:LEU:O	1:A:323:LEU:HB2	2.14	0.48
1:C:140:ARG:HB3	1:C:140:ARG:CZ	2.44	0.48
1:B:76:THR:HG22	1:C:230:ASP:N	2.28	0.48
1:A:75:TRP:CZ2	1:D:222:GLU:HB3	2.49	0.47
1:C:238:GLY:O	1:C:240:VAL:N	2.47	0.47
1:C:123:ARG:HB3	1:C:123:ARG:HH11	1.79	0.47
1:B:276:LEU:HD23	1:B:279:MET:HE3	1.97	0.47
1:C:132:ARG:O	1:C:136:VAL:HG13	2.13	0.47
1:D:374:MET:SD	1:D:375:THR:HG22	2.54	0.47
1:A:123:ARG:HH11	1:A:123:ARG:HB3	1.79	0.47
1:A:381:ASP:N	1:A:381:ASP:OD2	2.46	0.47
1:D:123:ARG:HH11	1:D:123:ARG:HB3	1.78	0.47
1:D:72:GLN:HE22	1:D:225:ASN:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:H	1:B:55:PRO:HD3	1.80	0.47
1:C:341:GLN:CA	1:C:341:GLN:HE21	2.25	0.47
1:B:217:SER:HA	1:B:220:LEU:HB2	1.97	0.47
1:C:262:TRP:HD1	1:C:273:GLU:OE2	1.97	0.47
1:C:319:LEU:HD22	1:C:487:PRO:HB3	1.97	0.47
1:D:443:CYS:HB2	3:D:600:HEM:C4A	2.50	0.47
1:A:94:HIS:ND1	1:A:382:ILE:HD12	2.29	0.47
1:B:218:GLY:HA2	1:B:221:ARG:CZ	2.45	0.47
1:B:345:PRO:HD3	1:B:462:GLN:HE22	1.80	0.47
1:C:350:GLN:NE2	1:C:357:THR:OG1	2.48	0.46
1:C:319:LEU:HB2	1:C:490:TYR:CE2	2.50	0.46
1:A:115:ARG:H	1:A:115:ARG:HG2	1.57	0.46
1:B:168:SER:C	1:B:170:ARG:H	2.19	0.46
1:B:291:ASN:HD22	1:B:293:GLU:HB2	1.80	0.46
1:D:103:PRO:HD3	1:D:123:ARG:HH21	1.80	0.46
1:D:114:PRO:HB2	1:D:115:ARG:CZ	2.45	0.46
1:C:170:ARG:CD	1:C:171:PRO:HD2	2.45	0.46
1:C:291:ASN:HD22	1:C:293:GLU:HB2	1.80	0.46
1:C:94:HIS:ND1	1:C:382:ILE:HD12	2.30	0.46
1:D:380:ARG:HA	1:D:391:LYS:HG3	1.96	0.46
1:C:208:LEU:HB3	1:C:247:PHE:HB2	1.96	0.46
1:A:41:PRO:C	1:D:221:ARG:HH21	2.18	0.46
1:A:333:GLN:HA	1:A:333:GLN:HE21	1.80	0.46
1:A:35:PRO:O	1:A:70:SER:HB2	2.16	0.46
1:B:388:ARG:NH1	1:B:388:ARG:HG2	2.26	0.46
1:B:149:LEU:HD13	1:B:448:LEU:HD13	1.98	0.46
1:C:150:GLU:O	1:C:154:THR:OG1	2.32	0.46
1:C:316:TRP:CD2	1:C:487:PRO:HG3	2.50	0.46
1:D:341:GLN:HA	1:D:341:GLN:HE21	1.81	0.46
1:B:227:VAL:CG2	1:C:227:VAL:HG21	2.46	0.46
1:C:149:LEU:HD13	1:C:448:LEU:HD13	1.97	0.46
1:C:321:MET:HE1	1:C:328:GLN:CA	2.46	0.46
1:B:129:ARG:O	1:B:133:ARG:HB2	2.15	0.45
1:C:319:LEU:O	1:C:323:LEU:HB2	2.16	0.45
1:C:89:GLU:O	1:C:93:THR:HB	2.16	0.45
1:B:250:GLN:HE21	1:B:250:GLN:HB3	1.59	0.45
1:A:175:ASN:ND2	1:A:175:ASN:H	2.15	0.45
1:A:262:TRP:CZ2	1:A:264:PRO:HA	2.51	0.45
1:A:416:HIS:NE2	1:A:418:GLU:HB2	2.31	0.45
1:C:34:PRO:CD	1:C:388:ARG:HH12	2.26	0.45
1:D:100:ASP:OD1	1:D:377:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:O	1:A:253:GLU:N	2.49	0.45
3:C:600:HEM:HBB2	3:C:600:HEM:HMB2	1.97	0.45
1:D:291:ASN:HD22	1:D:293:GLU:HB2	1.82	0.45
1:C:123:ARG:HH22	1:C:377:MET:HE1	1.82	0.45
1:D:474:ARG:HA	1:D:475:PRO:HD3	1.81	0.45
1:A:132:ARG:O	1:A:136:VAL:HG13	2.17	0.45
1:A:40:LEU:HD23	1:A:40:LEU:O	2.16	0.45
1:A:416:HIS:CD2	1:A:418:GLU:HB2	2.52	0.45
1:C:381:ASP:N	1:C:381:ASP:OD2	2.48	0.45
1:B:259:ARG:HE	1:B:276:LEU:HD22	1.82	0.45
1:D:150:GLU:O	1:D:154:THR:OG1	2.34	0.45
1:D:230:ASP:C	1:D:232:HIS:H	2.21	0.45
1:B:333:GLN:HA	1:B:333:GLN:NE2	2.32	0.45
1:B:443:CYS:HB2	3:B:600:HEM:C4A	2.52	0.45
1:C:220:LEU:HA	1:C:220:LEU:HD23	1.85	0.45
1:B:227:VAL:HG21	1:C:227:VAL:CG2	2.47	0.45
1:C:54:THR:N	1:C:55:PRO:HD3	2.32	0.45
1:B:218:GLY:HA2	1:B:221:ARG:NH1	2.32	0.44
1:B:251:LEU:O	1:B:255:LEU:HG	2.16	0.44
1:C:307:MET:HG2	1:C:308:VAL:N	2.32	0.44
1:A:88:ARG:HB3	1:A:88:ARG:HH11	1.81	0.44
1:A:55:PRO:HD3	1:A:481:PHE:CE2	2.52	0.44
1:B:75:TRP:HH2	1:C:219:PHE:O	2.00	0.44
1:C:217:SER:HA	1:C:220:LEU:HB2	1.99	0.44
1:C:241:LEU:O	1:C:242:ARG:C	2.56	0.44
1:A:187:ALA:O	1:A:191:CYS:HB2	2.17	0.44
1:B:34:PRO:CD	1:B:388:ARG:HH12	2.30	0.44
1:C:474:ARG:HA	1:C:475:PRO:HD3	1.88	0.44
1:B:187:ALA:O	1:B:191:CYS:N	2.48	0.44
1:B:287:GLU:O	1:B:288:SER:CB	2.50	0.44
1:D:178:LEU:O	1:D:182:VAL:HG23	2.17	0.44
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.52	0.44
1:D:67:ASP:O	1:D:82:ASN:HB2	2.18	0.44
1:C:257:GLU:HA	1:C:260:MET:HG2	2.00	0.44
1:A:150:GLU:O	1:A:154:THR:OG1	2.36	0.44
1:B:123:ARG:HH11	1:B:123:ARG:HB3	1.83	0.44
1:B:221:ARG:O	1:B:224:LEU:HG	2.18	0.44
1:C:279:MET:HB2	1:C:279:MET:HE2	1.92	0.44
1:D:114:PRO:HB2	1:D:115:ARG:NH1	2.32	0.44
1:A:474:ARG:HA	1:A:475:PRO:HD3	1.91	0.43
1:B:105:PRO:HD3	1:C:75:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ARG:NH2	1:D:374:MET:HG3	2.33	0.43
1:A:251:LEU:O	1:A:255:LEU:HG	2.17	0.43
1:A:294:ASN:O	1:A:298:VAL:HG23	2.17	0.43
1:D:466:PHE:HA	1:D:493:CYS:O	2.18	0.43
1:A:114:PRO:HB2	1:A:115:ARG:NH1	2.33	0.43
1:A:123:ARG:HH22	1:A:377:MET:HE1	1.83	0.43
1:B:114:PRO:HB2	1:B:115:ARG:NH2	2.32	0.43
1:C:333:GLN:HE21	1:C:333:GLN:HA	1.83	0.43
1:A:101:ARG:HA	1:A:102:PRO:HD3	1.91	0.43
1:B:380:ARG:HA	1:B:391:LYS:HG3	2.00	0.43
1:D:380:ARG:O	1:D:382:ILE:HG12	2.19	0.43
1:A:149:LEU:HD21	1:A:189:LEU:HD13	2.01	0.43
1:B:150:GLU:O	1:B:154:THR:OG1	2.36	0.43
1:C:229:VAL:C	1:C:231:ARG:N	2.70	0.43
1:D:132:ARG:NH2	1:D:442:ALA:O	2.27	0.43
1:B:149:LEU:HD21	1:B:189:LEU:HD13	2.01	0.43
1:B:323:LEU:HD13	1:B:475:PRO:HD2	2.01	0.43
1:B:132:ARG:NH2	1:B:442:ALA:O	2.36	0.43
1:C:461:LEU:HD23	1:C:466:PHE:CE1	2.54	0.43
1:B:445:GLY:O	1:B:446:GLU:C	2.57	0.43
3:B:600:HEM:CMB	3:B:600:HEM:HBB2	2.48	0.43
1:D:345:PRO:HD3	1:D:462:GLN:NE2	2.34	0.43
1:D:227:VAL:CG2	1:D:228:PRO:CD	2.85	0.43
1:B:170:ARG:CD	1:B:171:PRO:HD2	2.46	0.42
1:B:227:VAL:HB	1:C:227:VAL:HB	0.79	0.42
1:C:238:GLY:C	1:C:240:VAL:H	2.22	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.94	0.42
1:B:182:VAL:HG11	1:B:310:THR:HB	2.01	0.42
1:B:280:GLU:O	1:B:283:LYS:HG3	2.19	0.42
1:C:482:ALA:C	1:C:484:LEU:N	2.72	0.42
1:D:323:LEU:HD12	1:D:323:LEU:HA	1.86	0.42
1:A:221:ARG:O	1:A:224:LEU:HG	2.19	0.42
1:C:149:LEU:HD21	1:C:189:LEU:HD13	2.01	0.42
1:A:40:LEU:N	1:A:41:PRO:CD	2.81	0.42
1:A:371:PRO:HG2	1:A:481:PHE:CE1	2.54	0.42
1:C:173:ARG:HA	1:C:174:PRO:HD3	1.86	0.42
1:A:276:LEU:HD23	1:A:279:MET:HE3	2.00	0.42
1:B:294:ASN:HD22	1:B:294:ASN:HA	1.54	0.42
1:A:78:VAL:HG22	1:A:394:THR:HB	2.00	0.42
1:A:67:ASP:O	1:A:82:ASN:HB2	2.19	0.42
1:B:105:PRO:CD	1:C:75:TRP:CZ3	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:O	1:A:294:ASN:ND2	2.33	0.42
1:A:482:ALA:C	1:A:484:LEU:N	2.73	0.42
1:B:75:TRP:HZ2	1:C:219:PHE:HA	1.84	0.42
1:C:175:ASN:H	1:C:175:ASN:ND2	2.18	0.42
1:D:182:VAL:HG11	1:D:310:THR:HB	2.01	0.42
1:D:319:LEU:O	1:D:323:LEU:HB2	2.19	0.42
1:B:114:PRO:CB	1:B:115:ARG:NH2	2.83	0.42
1:A:149:LEU:O	1:A:153:VAL:HG23	2.19	0.42
1:C:129:ARG:HD3	1:C:440:ARG:HH22	1.85	0.42
1:D:285:ASN:HA	1:D:286:PRO:HD2	1.95	0.42
1:A:147:LYS:O	1:A:151:GLN:HB2	2.20	0.42
1:A:323:LEU:HA	1:A:323:LEU:HD12	1.80	0.42
1:A:481:PHE:O	1:A:481:PHE:CG	2.72	0.42
1:D:187:ALA:O	1:D:191:CYS:N	2.51	0.42
1:A:280:GLU:O	1:A:282:ALA:N	2.53	0.41
1:A:319:LEU:HB2	1:A:490:TYR:CE2	2.55	0.41
1:B:307:MET:HG2	1:B:308:VAL:N	2.34	0.41
1:B:481:PHE:O	1:B:481:PHE:CG	2.72	0.41
1:D:132:ARG:O	1:D:136:VAL:HG13	2.20	0.41
1:D:262:TRP:HD1	1:D:273:GLU:OE2	2.03	0.41
1:D:130:GLU:OE2	1:D:290:PHE:CE1	2.73	0.41
1:D:371:PRO:HG2	1:D:481:PHE:HE1	1.84	0.41
1:D:445:GLY:O	1:D:446:GLU:C	2.58	0.41
1:B:280:GLU:O	1:B:281:LYS:C	2.59	0.41
1:A:170:ARG:NH2	1:C:201:ARG:HH11	2.19	0.41
1:C:223:VAL:CG1	1:C:375:THR:HG21	2.50	0.41
1:C:416:HIS:HB3	1:C:419:HIS:CE1	2.56	0.41
1:C:67:ASP:O	1:C:82:ASN:HB2	2.20	0.41
1:A:54:THR:N	1:A:55:PRO:HD3	2.31	0.41
1:A:473:PRO:O	1:A:474:ARG:CB	2.61	0.41
1:A:132:ARG:NH1	1:A:441:ARG:HA	2.36	0.41
1:A:449:ALA:O	1:A:453:LEU:HG	2.21	0.41
1:C:143:GLY:O	1:C:144:LEU:HG	2.21	0.41
3:D:600:HEM:HBB2	3:D:600:HEM:HMB2	2.02	0.41
1:B:238:GLY:O	1:B:240:VAL:N	2.54	0.41
1:C:100:ASP:HA	1:C:124:TYR:HB2	2.03	0.41
1:C:482:ALA:C	1:C:484:LEU:H	2.24	0.41
1:D:410:GLU:O	1:D:411:LYS:HG3	2.21	0.41
1:A:458:THR:O	1:A:459:SER:C	2.58	0.41
1:B:285:ASN:HA	1:B:286:PRO:HD2	1.92	0.41
1:B:341:GLN:HE21	1:B:341:GLN:CA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:CZ2	1:C:264:PRO:HA	2.55	0.41
1:D:229:VAL:C	1:D:231:ARG:N	2.71	0.41
1:A:217:SER:HA	1:A:220:LEU:HB2	2.03	0.41
1:A:443:CYS:HB2	3:A:600:HEM:C4A	2.56	0.41
1:A:466:PHE:HA	1:A:493:CYS:O	2.21	0.41
1:C:128:TRP:CZ2	1:C:132:ARG:HD2	2.56	0.41
1:A:238:GLY:C	1:A:240:VAL:H	2.23	0.40
1:A:192:GLY:HA2	1:A:269:ARG:HH22	1.86	0.40
1:B:468:VAL:HA	1:B:469:PRO:HD3	1.97	0.40
1:B:75:TRP:CZ2	1:C:219:PHE:HA	2.55	0.40
1:C:323:LEU:HD13	1:C:475:PRO:HD2	2.03	0.40
1:B:173:ARG:HA	1:B:174:PRO:HD3	1.85	0.40
1:B:416:HIS:CD2	1:B:418:GLU:HB2	2.57	0.40
1:C:149:LEU:HA	1:C:149:LEU:HD23	1.92	0.40
1:C:331:VAL:HG13	1:C:356:THR:OG1	2.20	0.40
1:D:462:GLN:O	1:D:497:ARG:NH1	2.53	0.40
1:A:182:VAL:HG11	1:A:310:THR:HB	2.04	0.40
1:A:323:LEU:HD13	1:A:475:PRO:HD2	2.03	0.40
1:B:75:TRP:CZ3	1:C:105:PRO:HD3	2.57	0.40
1:C:323:LEU:HA	1:C:323:LEU:HD12	1.85	0.40
1:C:64:ARG:HG2	1:C:65:PHE:CD1	2.56	0.40
1:B:230:ASP:C	1:B:232:HIS:H	2.25	0.40
1:B:292:ASP:OD2	1:B:292:ASP:N	2.50	0.40
1:D:144:LEU:O	1:D:147:LYS:N	2.48	0.40
1:A:40:LEU:H	1:A:41:PRO:HD3	1.83	0.40
1:B:91:LEU:O	1:B:95:GLY:CA	2.70	0.40
1:B:38:LEU:HD22	1:C:240:VAL:CG2	2.52	0.40
1:D:238:GLY:C	1:D:240:VAL:H	2.24	0.40
1:D:294:ASN:HD22	1:D:294:ASN:HA	1.55	0.40
3:D:600:HEM:CBC	3:D:600:HEM:CMC	2.92	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	450/479 (94%)	396 (88%)	34 (8%)	20 (4%)	3	17
1	B	447/479 (93%)	397 (89%)	33 (7%)	17 (4%)	4	21
1	C	450/479 (94%)	397 (88%)	38 (8%)	15 (3%)	4	25
1	D	447/479 (93%)	395 (88%)	36 (8%)	16 (4%)	4	22
All	All	1794/1916 (94%)	1585 (88%)	141 (8%)	68 (4%)	4	21

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	40	LEU
1	A	114	PRO
1	A	145	GLY
1	A	229	VAL
1	A	230	ASP
1	A	239	LYS
1	B	35	PRO
1	B	229	VAL
1	B	230	ASP
1	C	35	PRO
1	C	40	LEU
1	C	112	PHE
1	C	229	VAL
1	C	230	ASP
1	C	239	LYS
1	D	35	PRO
1	D	145	GLY
1	D	229	VAL
1	D	230	ASP
1	A	112	PHE
1	A	252	ASP
1	B	145	GLY
1	B	239	LYS
1	B	392	GLY
1	D	112	PHE
1	D	239	LYS
1	A	225	ASN
1	A	228	PRO
1	A	281	LYS

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Mol	Chain	Res	Type
1	B	114	PRO
1	B	225	ASN
1	B	228	PRO
1	C	39	PRO
1	C	114	PRO
1	C	225	ASN
1	C	228	PRO
1	D	225	ASN
1	D	228	PRO
1	D	419	HIS
1	A	55	PRO
1	A	144	LEU
1	A	474	ARG
1	B	55	PRO
1	B	112	PHE
1	B	474	ARG
1	C	55	PRO
1	C	288	SER
1	C	392	GLY
1	C	474	ARG
1	D	55	PRO
1	D	288	SER
1	D	474	ARG
1	A	54	THR
1	A	288	SER
1	B	54	THR
1	B	288	SER
1	D	114	PRO
1	A	392	GLY
1	B	419	HIS
1	D	223	VAL
1	D	392	GLY
1	A	223	VAL
1	B	169	GLY
1	B	223	VAL
1	C	223	VAL
1	D	284	GLY
1	A	238	GLY

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	380/409 (93%)	330 (87%)	50 (13%)	5	20
1	B	377/409 (92%)	322 (85%)	55 (15%)	3	17
1	C	380/409 (93%)	328 (86%)	52 (14%)	4	19
1	D	377/409 (92%)	322 (85%)	55 (15%)	3	17
All	All	1514/1636 (92%)	1302 (86%)	212 (14%)	4	18

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	61	LEU
1	A	63	ARG
1	A	70	SER
1	A	71	LEU
1	A	88	ARG
1	A	101	ARG
1	A	116	SER
1	A	123	ARG
1	A	132	ARG
1	A	144	LEU
1	A	148	SER
1	A	154	THR
1	A	170	ARG
1	A	193	ARG
1	A	196	GLU
1	A	210	GLN
1	A	222	GLU
1	A	223	VAL
1	A	225	ASN
1	A	242	ARG
1	A	250	GLN
1	A	253	GLU
1	A	256	THR

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Mol	Chain	Res	Type
1	A	266	GLN
1	A	288	SER
1	A	291	ASN
1	A	292	ASP
1	A	294	ASN
1	A	296	ARG
1	A	307	MET
1	A	326	ASP
1	A	333	GLN
1	A	337	ASP
1	A	341	GLN
1	A	343	ARG
1	A	370	VAL
1	A	380	ARG
1	A	381	ASP
1	A	382	ILE
1	A	383	GLU
1	A	388	ARG
1	A	395	LEU
1	A	403	LEU
1	A	477	HIS
1	A	480	VAL
1	A	483	PHE
1	A	484	LEU
1	A	492	LEU
1	A	495	VAL
1	B	53	ASN
1	B	54	THR
1	B	63	ARG
1	B	70	SER
1	B	71	LEU
1	B	88	ARG
1	B	101	ARG
1	B	115	ARG
1	B	116	SER
1	B	123	ARG
1	B	130	GLU
1	B	132	ARG
1	B	133	ARG
1	B	137	SER
1	B	154	THR
1	B	170	ARG

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Mol	Chain	Res	Type
1	B	193	ARG
1	B	196	GLU
1	B	210	GLN
1	B	216	GLU
1	B	222	GLU
1	B	223	VAL
1	B	225	ASN
1	B	242	ARG
1	B	250	GLN
1	B	253	GLU
1	B	256	THR
1	B	266	GLN
1	B	283	LYS
1	B	291	ASN
1	B	292	ASP
1	B	294	ASN
1	B	296	ARG
1	B	304	SER
1	B	307	MET
1	B	326	ASP
1	B	333	GLN
1	B	337	ASP
1	B	341	GLN
1	B	343	ARG
1	B	370	VAL
1	B	380	ARG
1	B	381	ASP
1	B	382	ILE
1	B	388	ARG
1	B	395	LEU
1	B	403	LEU
1	B	440	ARG
1	B	477	HIS
1	B	480	VAL
1	B	483	PHE
1	B	484	LEU
1	B	488	SER
1	B	492	LEU
1	B	495	VAL
1	C	52	GLN
1	C	61	LEU
1	C	63	ARG

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Mol	Chain	Res	Type
1	C	70	SER
1	C	71	LEU
1	C	88	ARG
1	C	101	ARG
1	C	115	ARG
1	C	116	SER
1	C	123	ARG
1	C	130	GLU
1	C	132	ARG
1	C	136	VAL
1	C	144	LEU
1	C	154	THR
1	C	170	ARG
1	C	196	GLU
1	C	210	GLN
1	C	216	GLU
1	C	222	GLU
1	C	223	VAL
1	C	225	ASN
1	C	242	ARG
1	C	250	GLN
1	C	256	THR
1	C	266	GLN
1	C	288	SER
1	C	291	ASN
1	C	292	ASP
1	C	294	ASN
1	C	296	ARG
1	C	304	SER
1	C	307	MET
1	C	326	ASP
1	C	333	GLN
1	C	337	ASP
1	C	341	GLN
1	C	343	ARG
1	C	370	VAL
1	C	380	ARG
1	C	381	ASP
1	C	388	ARG
1	C	395	LEU
1	C	403	LEU
1	C	440	ARG

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Mol	Chain	Res	Type
1	C	477	HIS
1	C	480	VAL
1	C	483	PHE
1	C	484	LEU
1	C	488	SER
1	C	492	LEU
1	C	495	VAL
1	D	54	THR
1	D	63	ARG
1	D	70	SER
1	D	71	LEU
1	D	88	ARG
1	D	101	ARG
1	D	115	ARG
1	D	116	SER
1	D	123	ARG
1	D	130	GLU
1	D	132	ARG
1	D	133	ARG
1	D	137	SER
1	D	148	SER
1	D	154	THR
1	D	170	ARG
1	D	193	ARG
1	D	196	GLU
1	D	210	GLN
1	D	214	LYS
1	D	222	GLU
1	D	223	VAL
1	D	225	ASN
1	D	242	ARG
1	D	250	GLN
1	D	256	THR
1	D	266	GLN
1	D	283	LYS
1	D	288	SER
1	D	291	ASN
1	D	292	ASP
1	D	294	ASN
1	D	296	ARG
1	D	307	MET
1	D	326	ASP

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Mol	Chain	Res	Type
1	D	333	GLN
1	D	337	ASP
1	D	341	GLN
1	D	343	ARG
1	D	370	VAL
1	D	380	ARG
1	D	381	ASP
1	D	382	ILE
1	D	388	ARG
1	D	395	LEU
1	D	403	LEU
1	D	440	ARG
1	D	441	ARG
1	D	477	HIS
1	D	480	VAL
1	D	483	PHE
1	D	484	LEU
1	D	488	SER
1	D	492	LEU
1	D	495	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	60	GLN
1	A	72	GLN
1	A	166	ASN
1	A	175	ASN
1	A	250	GLN
1	A	291	ASN
1	A	333	GLN
1	A	341	GLN
1	A	350	GLN
1	A	477	HIS
1	B	53	ASN
1	B	166	ASN
1	B	175	ASN
1	B	225	ASN
1	B	244	GLN
1	B	250	GLN
1	B	291	ASN

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Mol	Chain	Res	Type
1	B	333	GLN
1	B	341	GLN
1	B	350	GLN
1	B	477	HIS
1	C	52	GLN
1	C	166	ASN
1	C	175	ASN
1	C	210	GLN
1	C	250	GLN
1	C	291	ASN
1	C	294	ASN
1	C	333	GLN
1	C	341	GLN
1	C	350	GLN
1	C	424	GLN
1	C	462	GLN
1	C	477	HIS
1	D	60	GLN
1	D	72	GLN
1	D	166	ASN
1	D	175	ASN
1	D	244	GLN
1	D	250	GLN
1	D	291	ASN
1	D	333	GLN
1	D	341	GLN
1	D	350	GLN
1	D	424	GLN
1	D	462	GLN
1	D	477	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	HEM	A	600	1	28,50,50	2.22	11 (39%)	17,82,82	1.75	5 (29%)
2	SO4	B	2000	-	4,4,4	0.36	0	6,6,6	1.05	0
2	SO4	B	2001	-	4,4,4	0.35	0	6,6,6	0.78	0
3	HEM	B	600	1	28,50,50	2.43	9 (32%)	17,82,82	1.50	3 (17%)
3	HEM	C	600	1	28,50,50	2.31	8 (28%)	17,82,82	1.82	5 (29%)
3	HEM	D	600	1	28,50,50	2.35	10 (35%)	17,82,82	1.50	6 (35%)

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
3	HEM	A	600	1	-	0/6/54/54	0/0/8/8
2	SO4	B	2000	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
3	HEM	B	600	1	-	0/6/54/54	0/0/8/8
3	HEM	C	600	1	-	0/6/54/54	0/0/8/8
3	HEM	D	600	1	-	0/6/54/54	0/0/8/8

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	HEM	C3C-C2C	-4.75	1.34	1.40
3	B	600	HEM	C3B-C2B	-4.47	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	HEM	C3B-C2B	-4.45	1.34	1.40
3	C	600	HEM	C3B-C2B	-4.00	1.35	1.40
3	C	600	HEM	C3C-C2C	-3.75	1.35	1.40
3	D	600	HEM	C3C-C2C	-3.44	1.35	1.40
3	A	600	HEM	C3B-C2B	-3.40	1.35	1.40
3	A	600	HEM	C3C-C2C	-2.54	1.37	1.40
3	D	600	HEM	C4D-ND	2.04	1.39	1.36
3	B	600	HEM	CMC-C2C	2.05	1.56	1.51
3	D	600	HEM	CMB-C2B	2.16	1.56	1.51
3	A	600	HEM	CAA-C2A	2.20	1.55	1.52
3	A	600	HEM	CMC-C2C	2.28	1.56	1.51
3	A	600	HEM	C4D-ND	2.33	1.39	1.36
3	D	600	HEM	CMC-C2C	2.50	1.56	1.51
3	A	600	HEM	C1C-NC	2.57	1.39	1.36
3	C	600	HEM	CAA-C2A	2.62	1.56	1.52
3	B	600	HEM	C4D-ND	3.26	1.40	1.36
3	A	600	HEM	C3B-CAB	3.31	1.54	1.47
3	B	600	HEM	CBB-CAB	3.43	1.53	1.28
3	D	600	HEM	CBB-CAB	3.48	1.53	1.28
3	A	600	HEM	CBB-CAB	3.52	1.53	1.28
3	B	600	HEM	CBC-CAC	3.53	1.53	1.28
3	C	600	HEM	CBB-CAB	3.54	1.53	1.28
3	D	600	HEM	CBC-CAC	3.56	1.53	1.28
3	C	600	HEM	CBC-CAC	3.65	1.54	1.28
3	B	600	HEM	C3C-CAC	3.70	1.55	1.47
3	A	600	HEM	CBC-CAC	3.74	1.55	1.28
3	A	600	HEM	C3C-CAC	3.78	1.55	1.47
3	C	600	HEM	C3C-CAC	4.17	1.56	1.47
3	D	600	HEM	C3B-CAB	4.18	1.56	1.47
3	D	600	HEM	C3C-CAC	4.20	1.56	1.47
3	C	600	HEM	C3D-C2D	4.45	1.50	1.37
3	B	600	HEM	C3B-CAB	4.55	1.56	1.47
3	C	600	HEM	C3B-CAB	4.70	1.57	1.47
3	D	600	HEM	C3D-C2D	4.88	1.52	1.37
3	A	600	HEM	C3D-C2D	5.24	1.53	1.37
3	B	600	HEM	C3D-C2D	5.40	1.53	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	HEM	C1D-C2D-C3D	-2.93	104.96	107.00
3	C	600	HEM	CMA-C3A-C4A	-2.86	124.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	HEM	CBD-CAD-C3D	-2.84	107.06	112.47
3	B	600	HEM	CAA-CBA-CGA	-2.69	108.06	112.66
3	D	600	HEM	C1D-C2D-C3D	-2.33	105.37	107.00
3	C	600	HEM	CAA-CBA-CGA	-2.20	108.91	112.66
3	D	600	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
3	A	600	HEM	C1D-C2D-C3D	-2.16	105.50	107.00
3	D	600	HEM	CBD-CAD-C3D	-2.12	108.42	112.47
3	B	600	HEM	CBD-CAD-C3D	-2.09	108.48	112.47
3	D	600	HEM	CAA-CBA-CGA	-2.08	109.10	112.66
3	D	600	HEM	CAD-CBD-CGD	-2.03	109.19	112.66
3	A	600	HEM	CMC-C2C-C3C	2.37	129.30	124.89
3	D	600	HEM	C4A-C3A-C2A	2.38	108.65	107.00
3	B	600	HEM	C4A-C3A-C2A	2.46	108.71	107.00
3	A	600	HEM	CMB-C2B-C3B	2.76	130.02	124.89
3	C	600	HEM	CMC-C2C-C3C	2.77	130.04	124.89
3	C	600	HEM	C4A-C3A-C2A	3.05	109.12	107.00
3	A	600	HEM	C4C-C3C-C2C	3.48	109.33	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	HEM	5	0
2	B	2000	SO4	2	0
3	B	600	HEM	6	0
3	C	600	HEM	5	0
3	D	600	HEM	8	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	454/479 (94%)	0.11	12 (2%) 56 27	50, 57, 63, 77	0
1	B	451/479 (94%)	0.25	20 (4%) 35 14	46, 57, 63, 71	0
1	C	454/479 (94%)	0.07	13 (2%) 52 24	49, 57, 63, 75	0
1	D	451/479 (94%)	0.20	23 (5%) 29 12	48, 57, 63, 72	0
All	All	1810/1916 (94%)	0.15	68 (3%) 41 17	46, 57, 63, 77	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	228	PRO	4.9
1	B	424	GLN	4.8
1	B	286	PRO	4.3
1	C	228	PRO	4.1
1	C	145	GLY	3.6
1	A	145	GLY	3.5
1	D	426	HIS	3.5
1	D	145	GLY	3.4
1	D	38	LEU	3.4
1	C	74	ALA	3.2
1	D	286	PRO	3.1
1	A	265	ALA	3.1
1	C	229	VAL	3.0
1	D	265	ALA	3.0
1	D	341	GLN	3.0
1	B	284	GLY	2.9
1	C	38	LEU	2.9
1	D	406	GLU	2.9
1	A	228	PRO	2.8
1	B	64	ARG	2.8
1	C	269	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	471	GLY	2.7
1	D	56	TYR	2.7
1	C	379	SER	2.7
1	D	39	PRO	2.7
1	C	75	TRP	2.7
1	A	496	PRO	2.6
1	B	426	HIS	2.6
1	B	74	ALA	2.6
1	D	424	GLN	2.5
1	B	354	PRO	2.5
1	A	341	GLN	2.5
1	D	495	VAL	2.4
1	D	228	PRO	2.4
1	C	423	ALA	2.4
1	D	146	LYS	2.4
1	C	77	PRO	2.3
1	D	340	GLY	2.3
1	C	146	LYS	2.3
1	A	146	LYS	2.3
1	B	285	ASN	2.3
1	A	60	GLN	2.3
1	D	64	ARG	2.2
1	D	423	ALA	2.2
1	B	425	GLY	2.2
1	B	231	ARG	2.2
1	A	56	TYR	2.2
1	A	380	ARG	2.2
1	A	235	ALA	2.1
1	B	66	GLY	2.1
1	D	285	ASN	2.1
1	D	70	SER	2.1
1	A	268	PRO	2.1
1	A	411	LYS	2.1
1	D	82	ASN	2.1
1	D	284	GLY	2.1
1	B	238	GLY	2.1
1	B	264	PRO	2.1
1	C	64	ARG	2.1
1	B	75	TRP	2.1
1	B	386	GLY	2.0
1	C	236	LEU	2.0
1	B	60	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	230	ASP	2.0
1	D	410	GLU	2.0
1	D	422	ASP	2.0
1	D	37	PRO	2.0
1	B	56	TYR	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	HEM	A	600	43/43	0.95	0.23	0.04	48,52,55,56	0
3	HEM	B	600	43/43	0.95	0.22	-0.19	48,52,55,56	0
3	HEM	D	600	43/43	0.96	0.19	-0.81	48,52,55,56	0
3	HEM	C	600	43/43	0.97	0.19	-1.18	48,52,55,56	0
2	SO4	B	2001	5/5	0.92	0.18	-1.83	52,54,57,58	0
2	SO4	B	2000	5/5	0.97	0.13	-2.68	46,51,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.