



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GQS  
Title : Structure of Human Microsomal Cytochrome P450 (CYP) 2C19  
Authors : Reynald, R.L.; Sansen, S.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2012-08-23  
Resolution : 2.87 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](mailto: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.

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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

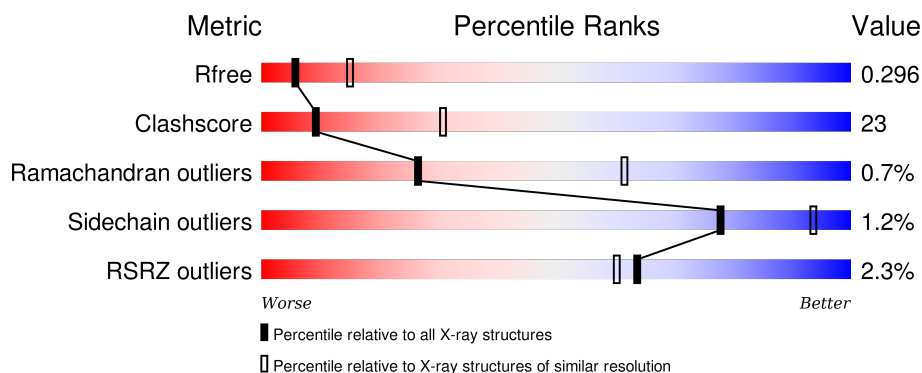
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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  $\geq 3$ , 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	477	 61% 35% 2% 4%
1	B	477	 51% 42% 2% 5%
1	C	477	 54% 42% 2% 4%
1	D	477	 53% 42% 5% 2%

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	0XV	C	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15043 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 2C19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3735	2400	635	677	23			
1	B	456	Total	C	N	O	S	0	0	0
			3666	2354	623	666	23			
1	C	462	Total	C	N	O	S	0	0	0
			3707	2384	627	673	23			
1	D	452	Total	C	N	O	S	0	0	0
			3611	2319	611	659	22			

There are 40 discrepancies between the modelled and reference sequences:

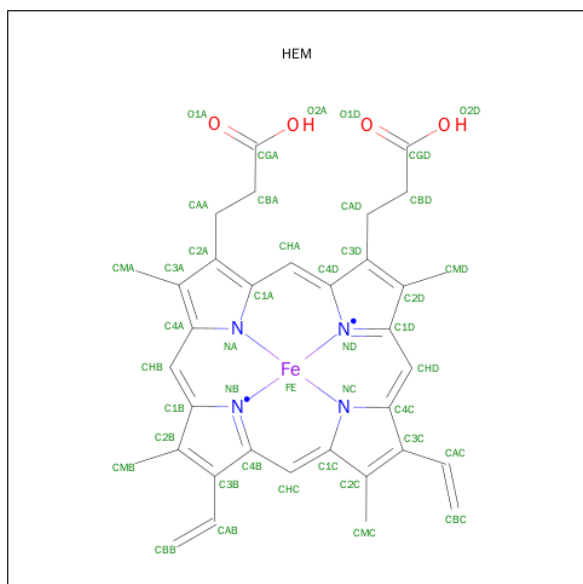
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP P33261
A	19	ALA	-	EXPRESSION TAG	UNP P33261
A	20	LYS	-	EXPRESSION TAG	UNP P33261
A	21	LYS	-	EXPRESSION TAG	UNP P33261
A	22	THR	-	EXPRESSION TAG	UNP P33261
A	490	ILE	-	EXPRESSION TAG	UNP P33261
A	491	HIS	-	EXPRESSION TAG	UNP P33261
A	492	HIS	-	EXPRESSION TAG	UNP P33261
A	493	HIS	-	EXPRESSION TAG	UNP P33261
A	494	HIS	-	EXPRESSION TAG	UNP P33261
B	18	MET	-	EXPRESSION TAG	UNP P33261
B	19	ALA	-	EXPRESSION TAG	UNP P33261
B	20	LYS	-	EXPRESSION TAG	UNP P33261
B	21	LYS	-	EXPRESSION TAG	UNP P33261
B	22	THR	-	EXPRESSION TAG	UNP P33261
B	490	ILE	-	EXPRESSION TAG	UNP P33261
B	491	HIS	-	EXPRESSION TAG	UNP P33261
B	492	HIS	-	EXPRESSION TAG	UNP P33261
B	493	HIS	-	EXPRESSION TAG	UNP P33261
B	494	HIS	-	EXPRESSION TAG	UNP P33261
C	18	MET	-	EXPRESSION TAG	UNP P33261

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Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ALA	-	EXPRESSION TAG	UNP P33261
C	20	LYS	-	EXPRESSION TAG	UNP P33261
C	21	LYS	-	EXPRESSION TAG	UNP P33261
C	22	THR	-	EXPRESSION TAG	UNP P33261
C	490	ILE	-	EXPRESSION TAG	UNP P33261
C	491	HIS	-	EXPRESSION TAG	UNP P33261
C	492	HIS	-	EXPRESSION TAG	UNP P33261
C	493	HIS	-	EXPRESSION TAG	UNP P33261
C	494	HIS	-	EXPRESSION TAG	UNP P33261
D	18	MET	-	EXPRESSION TAG	UNP P33261
D	19	ALA	-	EXPRESSION TAG	UNP P33261
D	20	LYS	-	EXPRESSION TAG	UNP P33261
D	21	LYS	-	EXPRESSION TAG	UNP P33261
D	22	THR	-	EXPRESSION TAG	UNP P33261
D	490	ILE	-	EXPRESSION TAG	UNP P33261
D	491	HIS	-	EXPRESSION TAG	UNP P33261
D	492	HIS	-	EXPRESSION TAG	UNP P33261
D	493	HIS	-	EXPRESSION TAG	UNP P33261
D	494	HIS	-	EXPRESSION TAG	UNP P33261

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



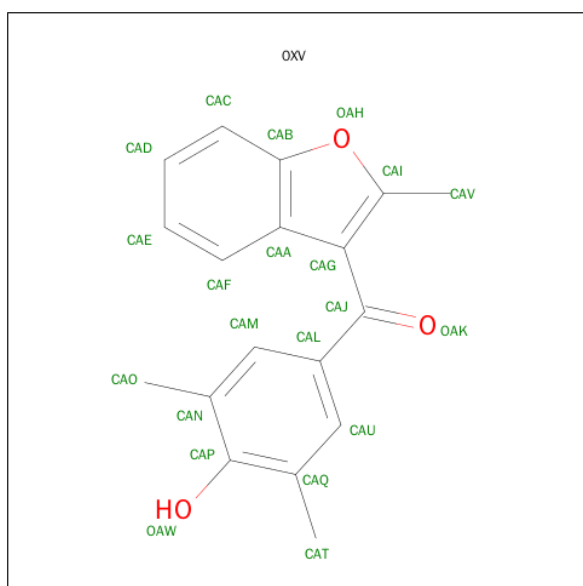
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is (4-HYDROXY-3,5-DIMETHYLPHENYL)(2-METHYL-1-BENZOFURAN-3-YL)METHANONE (three-letter code: 0XV) (formula: C<sub>18</sub>H<sub>16</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	18	3		
3	B	1	Total	C	O	0	0
			21	18	3		
3	C	1	Total	C	O	0	0
			21	18	3		
3	D	1	Total	C	O	0	0
			21	18	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

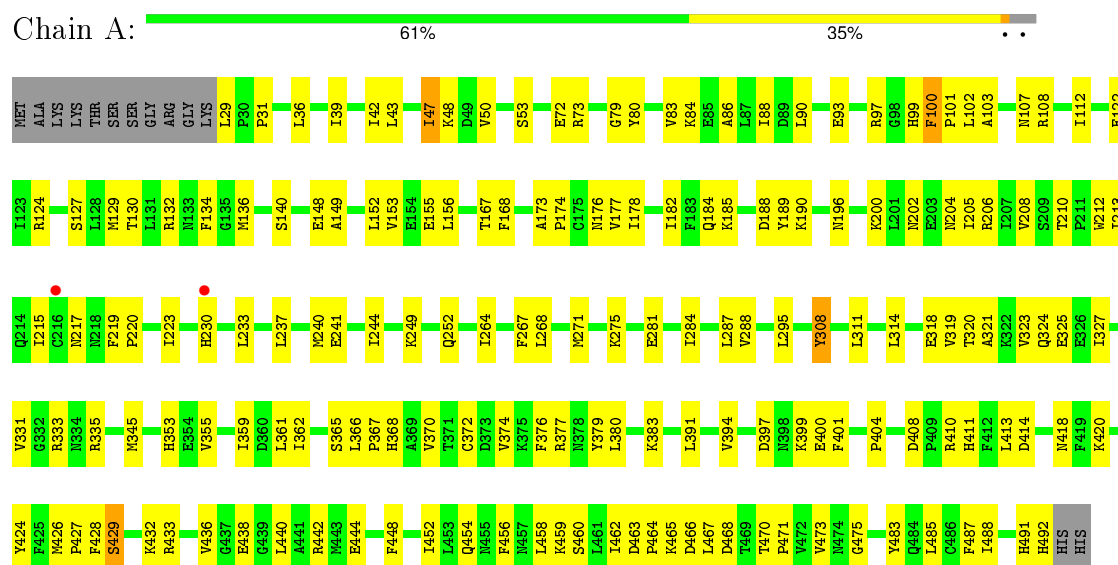
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	13	Total	O	0	0
			13	13		
5	C	12	Total	O	0	0
			12	12		
5	D	7	Total	O	0	0
			7	7		

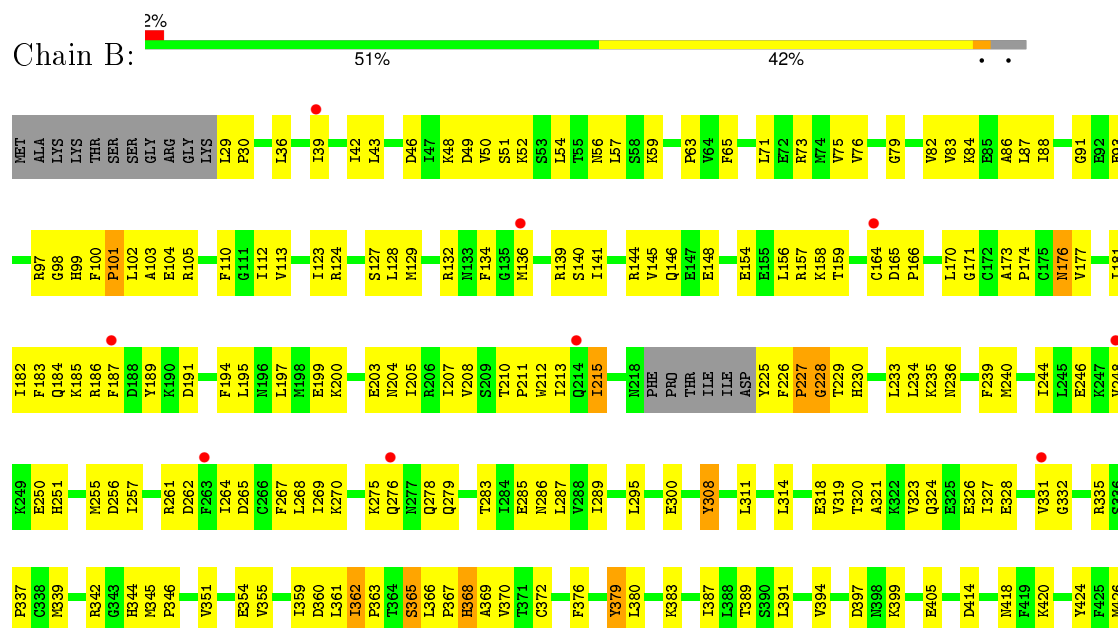
### 3 Residue-property plots

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 2C19



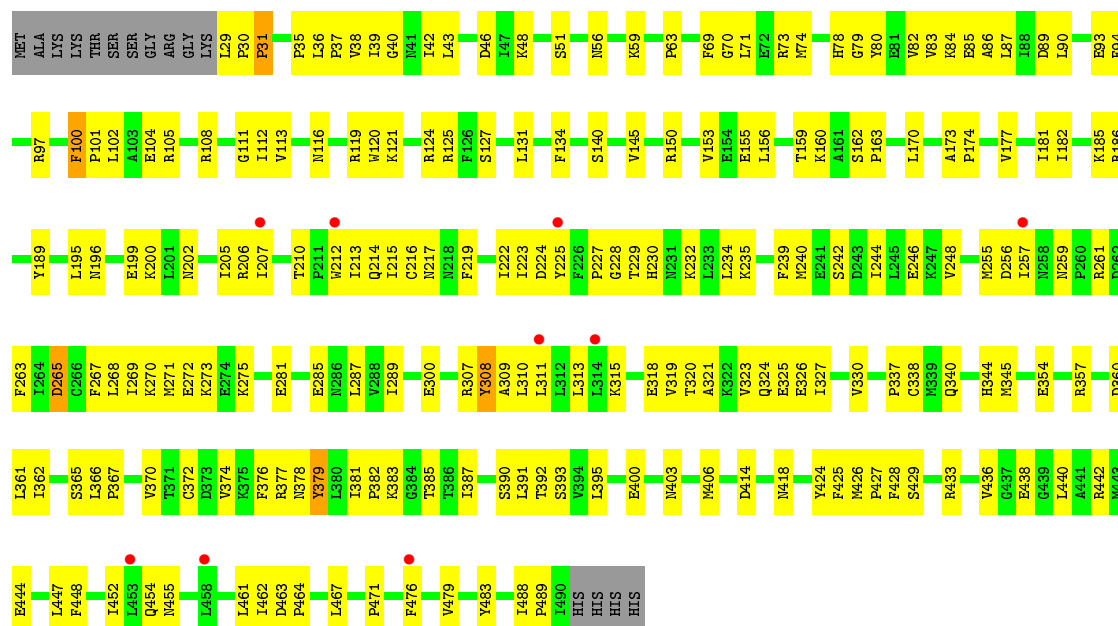
#### • Molecule 1: Cytochrome P450 2C19



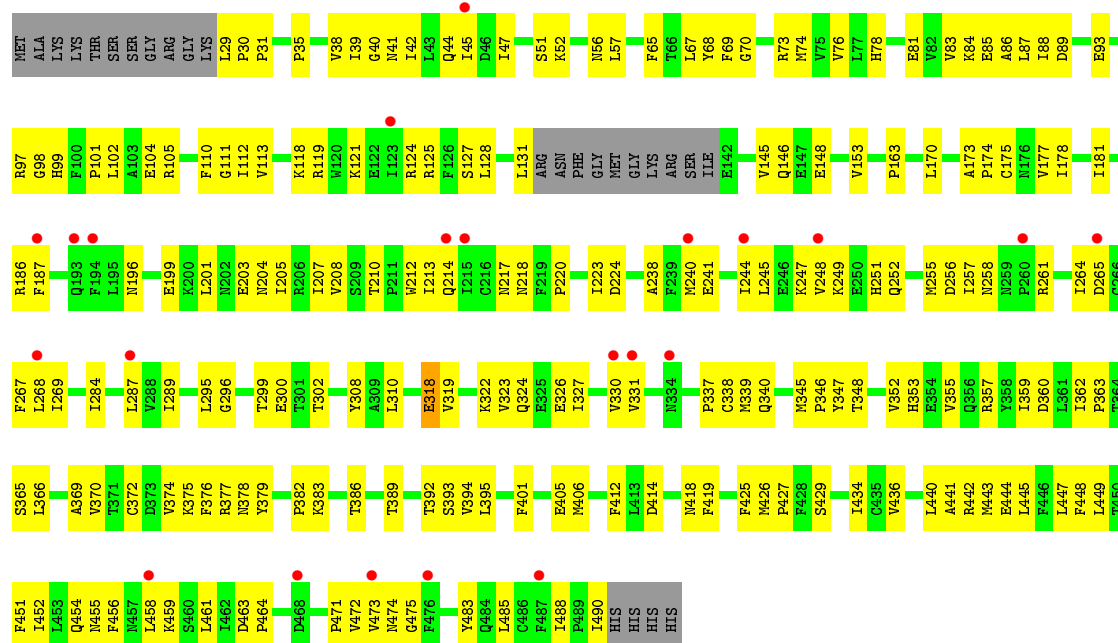




• Molecule 1: Cytochrome P450 2C19



• Molecule 1: Cytochrome P450 2C19



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.19Å 159.19Å 450.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.60 – 2.87 79.59 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.60-2.87) 99.9 (79.59-2.87)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.77 (at 2.86Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.250 , 0.296 0.245 , 0.296	Depositor DCC
$R_{free}$ test set	2574 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 74.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 50604 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 0XV, 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	0.26	0/3822	0.48	0/5172
1	B	0.26	0/3748	0.46	0/5068
1	C	0.27	0/3792	0.46	0/5132
1	D	0.26	0/3692	0.46	0/4999
All	All	0.26	0/15054	0.46	0/20371

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3735	0	3761	158	0
1	B	3666	0	3697	193	0
1	C	3707	0	3735	171	0
1	D	3611	0	3622	169	0
2	A	43	0	30	1	0
2	B	43	0	30	4	0
2	C	43	0	30	0	0
2	D	43	0	30	3	0
3	A	21	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	16	2	0
3	C	21	0	16	1	0
3	D	21	0	16	1	0
4	A	18	0	24	3	0
5	A	18	0	0	2	0
5	B	13	0	0	2	0
5	C	12	0	0	3	0
5	D	7	0	0	1	0
All	All	15043	0	15023	688	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 23.

All (688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HG3	1:A:88:ILE:HD12	1.36	1.06
1:D:163:PRO:HB3	1:D:461:LEU:HD21	1.42	0.98
1:C:63:PRO:HB2	1:C:82:VAL:HG21	1.48	0.95
1:B:52:LYS:HE2	5:B:613:HOH:O	1.68	0.92
1:B:200:LYS:HG2	1:B:236:ASN:HD22	1.36	0.90
1:D:87:LEU:HD21	1:D:389:THR:HG21	1.56	0.88
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.59	0.84
1:C:462:ILE:HG13	1:C:463:ASP:H	1.45	0.82
1:C:269:ILE:HG22	1:C:273:LYS:HE3	1.61	0.82
1:D:45:ILE:HD11	1:D:57:LEU:HD11	1.62	0.81
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.60	0.81
1:C:310:LEU:HA	1:C:313:LEU:HD12	1.63	0.80
1:A:467:LEU:HD12	1:A:467:LEU:O	1.82	0.80
1:B:257:ILE:HD12	1:B:257:ILE:H	1.47	0.80
1:D:112:ILE:HD11	1:D:436:VAL:HG21	1.64	0.79
1:C:214:GLN:NE2	1:C:476:PHE:H	1.81	0.78
1:A:101:PRO:HG2	1:A:217:ASN:O	1.84	0.78
1:C:170:LEU:HD11	1:C:310:LEU:HD12	1.64	0.78
1:D:324:GLN:HA	1:D:327:ILE:HD12	1.65	0.78
1:D:39:ILE:HB	1:D:42:ILE:HG12	1.65	0.78
1:A:268:LEU:HD23	1:A:271:MET:HE3	1.64	0.77
1:C:46:ASP:OD2	1:C:48:LYS:HB3	1.86	0.76
1:B:285:GLU:HB2	5:B:611:HOH:O	1.87	0.75
1:C:112:ILE:HD11	1:C:436:VAL:HG21	1.69	0.75
1:D:455:ASN:HA	1:D:490:ILE:HG12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:MET:HG2	1:B:256:ASP:H	1.52	0.75
1:D:148:GLU:HG2	1:D:177:VAL:HG23	1.70	0.74
1:D:39:ILE:O	1:D:70:GLY:HA2	1.89	0.73
1:A:268:LEU:HA	1:A:271:MET:HE2	1.68	0.73
1:B:251:HIS:HA	1:B:261:ARG:HH22	1.54	0.73
1:C:448:PHE:O	1:C:452:ILE:HG12	1.88	0.72
1:B:166:PRO:HB2	1:B:170:LEU:HD12	1.71	0.72
1:B:36:LEU:HD22	1:B:39:ILE:HD11	1.70	0.72
1:A:314:LEU:HD13	1:A:460:SER:HB3	1.70	0.72
1:B:101:PRO:O	1:B:104:GLU:HG2	1.90	0.72
1:C:185:LYS:HG2	1:C:186:ARG:H	1.55	0.72
1:C:479:VAL:CG1	5:C:612:HOH:O	2.37	0.72
1:C:121:LYS:O	1:C:125:ARG:HG2	1.90	0.72
1:D:173:ALA:HB3	1:D:174:PRO:HD3	1.73	0.71
1:C:101:PRO:HG2	1:C:217:ASN:O	1.92	0.70
1:B:283:THR:HG23	1:B:286:ASN:H	1.56	0.70
1:B:71:LEU:HD23	1:B:71:LEU:H	1.57	0.70
1:C:268:LEU:HD23	1:C:271:MET:HE3	1.73	0.70
1:C:173:ALA:HB3	1:C:174:PRO:HD3	1.74	0.70
1:C:56:ASN:HA	1:C:59:LYS:HD2	1.74	0.70
1:B:39:ILE:HD12	1:B:43:LEU:HD13	1.74	0.69
1:C:257:ILE:H	1:C:257:ILE:HD12	1.55	0.69
1:D:47:ILE:HD12	1:D:47:ILE:H	1.57	0.69
1:A:129:MET:HA	1:A:132:ARG:CD	2.22	0.68
1:A:468:ASP:OD2	1:A:470:THR:HB	1.93	0.68
1:A:397:ASP:OD2	1:A:399:LYS:HB3	1.94	0.68
1:C:272:GLU:HA	1:C:275:LYS:HE3	1.76	0.68
1:C:370:VAL:HG13	1:C:387:ILE:HD11	1.75	0.67
1:B:98:GLY:HA2	1:B:369:ALA:HB2	1.75	0.67
1:B:267:PHE:CE2	1:B:287:LEU:HB2	2.29	0.67
1:B:200:LYS:HG2	1:B:236:ASN:ND2	2.08	0.67
1:A:212:TRP:HA	1:A:215:ILE:HD12	1.76	0.67
1:C:270:LYS:HA	1:C:273:LYS:HD2	1.77	0.67
1:A:100:PHE:HE1	1:A:367:PRO:HG2	1.60	0.66
1:A:491:HIS:O	1:A:492:HIS:HB2	1.95	0.66
1:D:251:HIS:HA	1:D:261:ARG:HH21	1.61	0.66
1:A:90:LEU:O	1:A:93:GLU:HG2	1.95	0.66
1:A:215:ILE:HA	4:A:505:GOL:O2	1.95	0.66
1:B:366:LEU:HG	3:B:502:OXV:H2	1.78	0.66
1:D:366:LEU:HG	3:D:502:OXV:H2	1.77	0.65
1:B:311:LEU:HG	1:B:469:THR:HG22	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:VAL:HG13	5:C:612:HOH:O	1.95	0.65
1:D:146:GLN:HG2	1:D:447:LEU:HD13	1.79	0.65
1:A:223:ILE:HD11	1:A:230:HIS:HB2	1.78	0.65
1:D:110:PHE:HA	1:D:119:ARG:NH1	2.11	0.65
1:B:197:LEU:HD11	1:B:295:LEU:HD21	1.77	0.65
1:D:39:ILE:HD12	1:D:42:ILE:HD11	1.78	0.65
1:B:204:ASN:O	1:B:207:ILE:HG22	1.96	0.65
1:D:173:ALA:O	1:D:177:VAL:HG23	1.97	0.64
1:D:326:GLU:O	1:D:330:VAL:HG22	1.98	0.64
1:A:365:SER:HB2	1:A:391:LEU:HD11	1.80	0.64
1:D:178:ILE:HG21	1:D:295:LEU:HA	1.80	0.64
1:D:426:MET:N	1:D:427:PRO:HD3	2.12	0.64
1:C:202:ASN:O	1:C:206:ARG:HG3	1.98	0.64
1:C:29:LEU:HD11	1:C:73:ARG:CZ	2.28	0.63
1:C:102:LEU:HD11	1:C:213:ILE:HG23	1.80	0.63
1:B:351:VAL:O	1:B:355:VAL:HG23	1.99	0.63
1:D:207:ILE:HG22	1:D:213:ILE:HD12	1.80	0.63
1:A:473:VAL:HG12	1:A:475:GLY:H	1.62	0.63
1:D:459:LYS:HA	1:D:459:LYS:NZ	2.13	0.63
1:C:426:MET:N	1:C:427:PRO:HD3	2.13	0.63
1:B:46:ASP:OD2	1:B:48:LYS:HG2	1.99	0.63
1:D:214:GLN:HE22	1:D:475:GLY:HA2	1.62	0.63
1:C:214:GLN:HE22	1:C:476:PHE:H	1.45	0.63
1:D:319:VAL:O	1:D:323:VAL:HG23	1.99	0.63
1:D:203:GLU:O	1:D:207:ILE:HG12	1.99	0.63
1:C:267:PHE:CE2	1:C:287:LEU:HB2	2.34	0.63
1:D:98:GLY:HA2	1:D:369:ALA:HB2	1.81	0.62
1:D:323:VAL:O	1:D:327:ILE:HG13	1.99	0.62
1:A:93:GLU:O	1:A:370:VAL:HA	1.98	0.62
1:C:39:ILE:HB	1:C:42:ILE:HG12	1.81	0.62
1:B:50:VAL:HG13	1:B:51:SER:H	1.64	0.62
1:D:458:LEU:HB3	1:D:485:LEU:HD12	1.81	0.62
1:B:157:ARG:HG2	1:B:157:ARG:HH11	1.63	0.62
1:D:148:GLU:HA	1:D:148:GLU:OE2	1.98	0.62
1:D:256:ASP:OD1	1:D:258:ASN:HB2	1.99	0.62
1:B:211:PRO:O	1:B:215:ILE:HG12	1.98	0.62
1:A:458:LEU:HD22	1:A:485:LEU:HD12	1.80	0.62
1:D:267:PHE:CG	1:D:287:LEU:HD13	2.35	0.62
1:B:141:ILE:O	1:B:145:VAL:HG23	1.99	0.62
1:A:361:LEU:C	1:A:362:ILE:HD13	2.21	0.62
1:A:99:HIS:CE1	5:A:614:HOH:O	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:OD2	1:A:190:LYS:HB2	2.00	0.61
1:B:323:VAL:O	1:B:327:ILE:HG13	2.00	0.61
1:B:255:MET:HG2	1:B:256:ASP:N	2.14	0.61
1:B:204:ASN:OD1	1:B:233:LEU:HD12	2.00	0.61
1:A:155:GLU:HG3	1:A:189:TYR:CE1	2.35	0.61
1:A:333:ARG:HH11	1:A:333:ARG:HG3	1.66	0.61
1:B:397:ASP:OD2	1:B:399:LYS:HB2	2.01	0.61
1:B:63:PRO:HB2	1:B:82:VAL:HG11	1.81	0.61
1:D:87:LEU:HD21	1:D:389:THR:CG2	2.29	0.61
1:C:224:ASP:O	1:C:227:PRO:HD3	2.01	0.61
1:A:102:LEU:HD11	1:A:233:LEU:CD2	2.31	0.61
1:A:112:ILE:HD11	1:A:127:SER:OG	2.00	0.61
1:D:348:THR:O	1:D:352:VAL:HG23	2.01	0.60
1:D:472:VAL:HG12	1:D:474:ASN:H	1.65	0.60
1:D:318:GLU:OE2	1:D:319:VAL:HG23	1.99	0.60
1:A:102:LEU:HD11	1:A:233:LEU:HD23	1.84	0.60
1:B:251:HIS:HA	1:B:261:ARG:NH2	2.16	0.60
1:A:36:LEU:HD21	1:C:43:LEU:HD22	1.84	0.60
1:C:155:GLU:HG3	1:C:189:TYR:CD1	2.37	0.60
1:B:148:GLU:OE2	1:B:186:ARG:HD2	2.01	0.60
1:A:134:PHE:CE2	1:A:140:SER:HB3	2.36	0.60
1:B:362:ILE:HD12	1:B:362:ILE:H	1.67	0.60
1:C:185:LYS:HG2	1:C:186:ARG:N	2.16	0.60
1:D:121:LYS:HD3	1:D:125:ARG:NH2	2.17	0.59
1:A:426:MET:N	1:A:427:PRO:HD3	2.17	0.59
1:D:39:ILE:HB	1:D:42:ILE:CG1	2.31	0.59
1:A:267:PHE:CG	1:A:287:LEU:HD13	2.37	0.59
1:A:308:TYR:OH	1:A:471:PRO:HG3	2.02	0.59
1:B:207:ILE:HG21	1:B:233:LEU:HB2	1.85	0.59
1:C:464:PRO:HA	1:C:467:LEU:HD13	1.85	0.59
1:D:101:PRO:HG2	1:D:217:ASN:O	2.03	0.59
1:B:139:ARG:HH21	1:B:144:ARG:HA	1.68	0.59
1:B:128:LEU:HD12	1:B:436:VAL:HG13	1.85	0.59
1:B:87:LEU:HD11	1:B:368:HIS:CE1	2.38	0.59
1:C:79:GLY:O	1:C:83:VAL:HG23	2.03	0.59
1:A:167:THR:HG23	1:A:168:PHE:N	2.18	0.59
1:C:462:ILE:HG13	1:C:463:ASP:N	2.15	0.58
1:D:105:ARG:HH22	1:D:224:ASP:N	2.01	0.58
1:C:210:THR:O	1:C:214:GLN:HG3	2.03	0.58
1:C:156:LEU:HD11	1:C:452:ILE:HD12	1.84	0.58
1:A:90:LEU:HB3	1:A:93:GLU:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ALA:O	1:A:325:GLU:HG3	2.04	0.58
1:C:156:LEU:O	1:C:159:THR:HG22	2.03	0.58
1:B:244:ILE:O	1:B:248:VAL:HG23	2.02	0.58
1:C:100:PHE:O	1:C:104:GLU:HG2	2.02	0.58
1:B:171:GLY:O	1:B:174:PRO:HD2	2.03	0.58
1:C:155:GLU:HG3	1:C:189:TYR:CE1	2.38	0.58
1:C:36:LEU:HB3	1:C:37:PRO:HD2	1.85	0.58
1:A:323:VAL:O	1:A:327:ILE:HG13	2.04	0.58
1:C:223:ILE:HD11	1:C:230:HIS:ND1	2.19	0.58
1:D:148:GLU:HG2	1:D:177:VAL:CG2	2.33	0.57
1:A:129:MET:HA	1:A:132:ARG:HD2	1.84	0.57
1:A:36:LEU:CD2	1:A:39:ILE:HD11	2.33	0.57
1:D:39:ILE:O	1:D:70:GLY:CA	2.51	0.57
1:D:97:ARG:NH1	1:D:366:LEU:HB3	2.19	0.57
1:D:339:MET:SD	1:D:443:MET:HG3	2.44	0.57
1:C:101:PRO:HD2	1:C:217:ASN:ND2	2.20	0.57
1:B:365:SER:HB2	1:B:391:LEU:CD1	2.34	0.57
1:D:459:LYS:HA	1:D:459:LYS:HZ3	1.68	0.57
1:D:74:MET:HB3	1:D:386:THR:HB	1.86	0.57
1:C:381:ILE:N	1:C:381:ILE:HD12	2.20	0.57
1:C:244:ILE:O	1:C:248:VAL:HG23	2.04	0.57
1:B:191:ASP:O	1:B:195:LEU:HG	2.05	0.57
1:C:173:ALA:O	1:C:177:VAL:HG23	2.04	0.56
1:C:36:LEU:HB3	1:C:37:PRO:CD	2.35	0.56
1:A:414:ASP:OD2	1:A:418:ASN:HB2	2.05	0.56
1:A:249:LYS:HA	1:A:252:GLN:OE1	2.05	0.56
1:C:267:PHE:CG	1:C:287:LEU:HD13	2.40	0.56
1:D:127:SER:O	1:D:131:LEU:HD13	2.06	0.56
1:B:36:LEU:CD2	1:B:39:ILE:HD11	2.36	0.56
1:D:170:LEU:HD11	1:D:310:LEU:HD12	1.87	0.56
1:B:227:PRO:HG2	1:B:228:GLY:H	1.70	0.56
1:D:454:GLN:O	1:D:490:ILE:HD13	2.06	0.56
1:A:100:PHE:CE1	1:A:367:PRO:HG2	2.39	0.56
1:C:177:VAL:O	1:C:181:ILE:HG12	2.05	0.56
1:C:182:ILE:HA	1:C:263:PHE:HB3	1.87	0.56
1:A:240:MET:O	1:A:244:ILE:HG13	2.06	0.56
1:B:189:TYR:O	1:B:195:LEU:HD21	2.06	0.56
1:A:206:ARG:O	1:A:210:THR:HG23	2.05	0.56
1:C:196:ASN:HA	1:C:199:GLU:OE1	2.06	0.56
1:C:127:SER:O	1:C:131:LEU:HG	2.06	0.56
1:A:129:MET:O	1:A:132:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:SER:HB2	1:B:391:LEU:HD11	1.88	0.56
1:D:84:LYS:CG	1:D:88:ILE:HD12	2.36	0.56
1:B:104:GLU:HG3	1:B:105:ARG:N	2.21	0.56
1:D:441:ALA:O	1:D:445:LEU:HD23	2.06	0.56
1:B:187:PHE:CD1	1:B:194:PHE:HB2	2.41	0.55
1:B:240:MET:O	1:B:244:ILE:HG13	2.06	0.55
1:C:80:TYR:CZ	1:C:84:LYS:HD2	2.41	0.55
1:D:377:ARG:O	1:D:378:ASN:HB3	2.06	0.55
1:B:166:PRO:HB2	1:B:170:LEU:CD1	2.36	0.55
1:D:267:PHE:CE2	1:D:287:LEU:HB2	2.41	0.55
1:B:318:GLU:HG2	1:B:319:VAL:N	2.21	0.55
1:B:63:PRO:HB2	1:B:82:VAL:CG1	2.37	0.55
1:A:223:ILE:HD13	1:A:230:HIS:ND1	2.21	0.55
1:B:314:LEU:HD11	1:B:485:LEU:HD13	1.88	0.55
1:C:112:ILE:HG23	1:C:113:VAL:N	2.21	0.55
1:D:173:ALA:HB1	1:D:448:PHE:CE2	2.42	0.55
1:D:252:GLN:HA	1:D:268:LEU:HD21	1.88	0.55
1:B:100:PHE:HB3	1:B:103:ALA:HB3	1.89	0.55
1:A:284:ILE:O	1:A:288:VAL:HG23	2.07	0.55
1:D:39:ILE:HD12	1:D:42:ILE:CD1	2.36	0.55
1:D:73:ARG:HH11	1:D:73:ARG:HB3	1.72	0.55
1:C:200:LYS:HE3	1:C:240:MET:HB2	1.89	0.55
1:C:150:ARG:O	1:C:153:VAL:HG12	2.07	0.55
1:B:331:VAL:HG21	1:B:337:PRO:HB3	1.89	0.54
1:B:405:GLU:OE2	1:B:405:GLU:HA	2.08	0.54
1:D:175:CYS:HB2	1:D:299:THR:HG23	1.89	0.54
1:B:134:PHE:CZ	1:B:140:SER:HB2	2.42	0.54
1:A:353:HIS:HE1	1:A:442:ARG:HH22	1.55	0.54
1:A:130:THR:HG22	1:A:136:MET:HE2	1.89	0.54
1:B:372:CYS:HA	1:B:383:LYS:HB2	1.88	0.54
1:D:44:GLN:NE2	5:D:607:HOH:O	2.41	0.54
1:B:187:PHE:HB3	1:B:194:PHE:HB2	1.90	0.54
1:B:124:ARG:O	1:B:128:LEU:HD13	2.08	0.54
1:A:413:LEU:O	1:A:420:LYS:HE2	2.08	0.54
1:D:452:ILE:O	1:D:456:PHE:HB2	2.07	0.54
1:C:255:MET:HE1	1:C:257:ILE:HG13	1.90	0.54
1:A:90:LEU:HB3	1:A:93:GLU:HG2	1.90	0.54
1:D:436:VAL:O	1:D:436:VAL:HG12	2.07	0.54
1:B:362:ILE:HD12	1:B:362:ILE:N	2.23	0.54
1:A:267:PHE:CE2	1:A:287:LEU:HB2	2.42	0.54
1:C:71:LEU:O	1:C:71:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PRO:HG2	1:B:428:PHE:CD2	2.42	0.54
1:B:368:HIS:NE2	1:B:433:ARG:HB2	2.23	0.54
1:C:414:ASP:OD2	1:C:418:ASN:HB2	2.08	0.54
1:D:153:VAL:CG1	1:D:455:ASN:HD21	2.21	0.53
1:A:408:ASP:OD1	1:A:410:ARG:HD2	2.08	0.53
1:A:366:LEU:HG	3:A:502:OXV:H2	1.90	0.53
1:D:29:LEU:HD11	1:D:73:ARG:HE	1.73	0.53
1:C:361:LEU:HB3	1:C:362:ILE:HD12	1.89	0.53
1:C:265:ASP:O	1:C:269:ILE:HG13	2.07	0.53
1:B:157:ARG:HG2	1:B:157:ARG:NH1	2.24	0.53
1:A:122:GLU:HG3	1:A:281:GLU:HG3	1.91	0.53
1:D:186:ARG:HG2	1:D:187:PHE:N	2.23	0.53
1:A:394:VAL:HG21	1:A:426:MET:HE1	1.90	0.53
1:B:49:ASP:OD1	1:B:473:VAL:HG11	2.09	0.53
1:C:376:PHE:O	1:C:377:ARG:HG3	2.09	0.53
1:C:338:CYS:SG	1:C:340:GLN:HB2	2.48	0.53
1:D:196:ASN:O	1:D:199:GLU:HB3	2.09	0.53
1:C:51:SER:OG	1:C:392:THR:HG21	2.09	0.53
1:B:355:VAL:O	1:B:359:ILE:HG12	2.09	0.53
1:A:353:HIS:CE1	1:A:442:ARG:HH22	2.26	0.53
1:A:372:CYS:HA	1:A:383:LYS:HG3	1.89	0.53
1:C:131:LEU:HD12	1:C:436:VAL:HG12	1.90	0.53
1:C:156:LEU:CD1	1:C:452:ILE:HD12	2.39	0.53
1:A:361:LEU:O	1:A:362:ILE:HD13	2.09	0.52
1:A:79:GLY:O	1:A:83:VAL:HG23	2.09	0.52
1:D:355:VAL:O	1:D:359:ILE:HG23	2.08	0.52
1:A:167:THR:CG2	1:A:168:PHE:N	2.73	0.52
1:C:365:SER:HB2	1:C:391:LEU:HD11	1.91	0.52
1:D:442:ARG:HH11	1:D:442:ARG:HG2	1.75	0.52
1:B:84:LYS:O	1:B:88:ILE:HB	2.09	0.52
1:B:476:PHE:CG	1:B:477:ALA:N	2.78	0.52
1:C:134:PHE:CE2	1:C:140:SER:HB3	2.45	0.52
1:A:428:PHE:CD2	1:A:438:GLU:HG3	2.45	0.52
1:D:153:VAL:HG13	1:D:456:PHE:HE2	1.75	0.52
1:D:330:VAL:HG23	1:D:331:VAL:HG23	1.92	0.52
1:A:318:GLU:HG2	1:A:319:VAL:N	2.25	0.52
1:C:285:GLU:O	1:C:289:ILE:HD13	2.09	0.52
1:A:129:MET:SD	1:B:328:GLU:OE1	2.67	0.52
1:B:394:VAL:HG11	1:B:426:MET:CE	2.39	0.52
1:C:365:SER:OG	1:C:366:LEU:N	2.42	0.52
1:B:65:PHE:CE2	1:B:76:VAL:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.75	0.52
1:D:245:LEU:HD11	1:D:284:ILE:HD11	1.91	0.52
1:A:129:MET:HA	1:A:132:ARG:HD3	1.91	0.52
1:B:446:PHE:HD1	1:B:447:LEU:HD23	1.75	0.52
1:D:372:CYS:O	1:D:374:VAL:HG23	2.10	0.52
1:B:134:PHE:CE2	1:B:140:SER:HB2	2.45	0.51
1:B:82:VAL:HG23	1:B:83:VAL:N	2.25	0.51
1:C:100:PHE:CD2	1:C:367:PRO:HG2	2.46	0.51
1:A:220:PRO:O	1:A:223:ILE:HG22	2.11	0.51
1:C:100:PHE:HD2	1:C:367:PRO:HG2	1.75	0.51
1:B:199:GLU:O	1:B:203:GLU:HB2	2.11	0.51
1:A:462:ILE:HD12	1:A:463:ASP:O	2.10	0.51
1:A:100:PHE:HB3	1:A:103:ALA:HB3	1.92	0.51
1:C:86:ALA:HB2	1:C:376:PHE:CE1	2.45	0.51
1:D:463:ASP:OD1	1:D:464:PRO:HD2	2.10	0.51
1:B:39:ILE:HB	1:B:42:ILE:CG2	2.41	0.51
1:B:50:VAL:HG13	1:B:51:SER:N	2.25	0.51
1:B:139:ARG:NH2	1:B:144:ARG:HA	2.26	0.51
1:B:257:ILE:H	1:B:257:ILE:CD1	2.20	0.51
1:B:257:ILE:HD12	1:B:257:ILE:N	2.22	0.51
1:B:361:LEU:HB3	1:B:362:ILE:HD12	1.93	0.51
1:A:320:THR:O	1:A:324:GLN:HG3	2.10	0.51
1:C:223:ILE:HD11	1:C:230:HIS:CG	2.45	0.51
1:D:145:VAL:HG21	1:D:443:MET:SD	2.50	0.51
1:D:445:LEU:O	1:D:449:LEU:HB2	2.10	0.51
1:D:440:LEU:O	1:D:444:GLU:HG3	2.10	0.51
1:D:310:LEU:HB2	1:D:483:TYR:OH	2.11	0.51
1:D:318:GLU:O	1:D:322:LYS:HG3	2.10	0.50
1:C:326:GLU:HG2	1:C:345:MET:HG2	1.92	0.50
1:A:462:ILE:HD11	1:A:467:LEU:HB3	1.92	0.50
1:B:113:VAL:HG21	3:B:502:OXV:H10	1.93	0.50
1:D:395:LEU:HD21	1:D:426:MET:H	1.76	0.50
1:A:80:TYR:OH	1:A:84:LYS:HD3	2.11	0.50
1:D:330:VAL:HG21	1:D:345:MET:HG2	1.93	0.50
1:B:361:LEU:O	1:B:363:PRO:HD3	2.11	0.50
1:D:73:ARG:HH11	1:D:73:ARG:CB	2.24	0.50
1:D:205:ILE:HG13	1:D:300:GLU:HG2	1.93	0.50
1:A:208:VAL:HA	1:A:213:ILE:HG21	1.92	0.50
1:A:237:LEU:HB3	1:A:241:GLU:OE2	2.12	0.50
1:D:73:ARG:NH1	1:D:73:ARG:HB3	2.27	0.50
1:A:130:THR:HG22	1:A:136:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ILE:HG12	1:C:345:MET:HE1	1.93	0.50
1:B:275:LYS:HG2	1:B:276:GLN:N	2.26	0.50
1:A:202:ASN:O	1:A:205:ILE:HG22	2.11	0.50
1:D:257:ILE:HG13	1:D:258:ASN:N	2.27	0.50
1:B:128:LEU:CD1	1:B:436:VAL:HG13	2.41	0.50
1:A:448:PHE:O	1:A:452:ILE:HG13	2.11	0.50
1:C:390:SER:OG	1:C:393:SER:HB3	2.12	0.50
1:A:36:LEU:HD23	1:A:39:ILE:HD11	1.93	0.50
1:D:84:LYS:HG3	1:D:88:ILE:HD12	1.94	0.50
1:D:81:GLU:O	1:D:85:GLU:HG3	2.11	0.50
1:C:195:LEU:O	1:C:199:GLU:HG3	2.12	0.49
1:D:414:ASP:OD1	1:D:418:ASN:N	2.40	0.49
1:D:177:VAL:O	1:D:181:ILE:HG13	2.12	0.49
1:B:87:LEU:HD21	1:B:389:THR:HG21	1.94	0.49
1:C:93:GLU:O	1:C:370:VAL:HA	2.12	0.49
1:C:268:LEU:HD23	1:C:271:MET:CE	2.42	0.49
1:C:39:ILE:O	1:C:42:ILE:HG12	2.13	0.49
1:B:327:ILE:HA	1:B:345:MET:HE3	1.94	0.49
1:B:29:LEU:HD23	1:B:380:LEU:O	2.13	0.49
1:C:207:ILE:O	1:C:210:THR:HG22	2.12	0.49
1:B:283:THR:HG22	1:B:286:ASN:HB2	1.95	0.49
1:A:467:LEU:HD12	1:A:467:LEU:C	2.33	0.49
1:A:365:SER:HB2	1:A:391:LEU:CD1	2.43	0.49
1:B:176:ASN:OD1	1:B:186:ARG:HG2	2.13	0.49
1:B:105:ARG:HH11	1:B:234:LEU:HD22	1.78	0.49
1:B:145:VAL:HG21	1:B:443:MET:SD	2.53	0.49
1:A:155:GLU:HG3	1:A:189:TYR:HE1	1.78	0.49
1:B:428:PHE:O	1:B:429:SER:HB3	2.13	0.49
1:B:93:GLU:N	1:B:93:GLU:OE2	2.46	0.49
1:D:363:PRO:HB3	1:D:392:THR:HG1	1.78	0.49
1:D:338:CYS:SG	1:D:340:GLN:HB2	2.53	0.48
1:D:394:VAL:HG11	1:D:426:MET:SD	2.52	0.48
1:B:446:PHE:O	1:B:450:THR:HG23	2.13	0.48
1:B:269:ILE:HG22	1:B:270:LYS:N	2.28	0.48
1:B:101:PRO:HG2	1:B:102:LEU:H	1.78	0.48
1:B:29:LEU:HD11	1:B:73:ARG:NH1	2.28	0.48
1:B:177:VAL:O	1:B:181:ILE:HG13	2.12	0.48
1:C:177:VAL:HG11	1:C:440:LEU:HD11	1.95	0.48
1:A:264:ILE:HG22	1:A:268:LEU:HD12	1.95	0.48
1:D:244:ILE:O	1:D:248:VAL:HG23	2.12	0.48
1:C:163:PRO:HB3	1:C:461:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LEU:CD2	1:D:426:MET:H	2.26	0.48
1:B:82:VAL:HG23	1:B:83:VAL:H	1.77	0.48
1:D:363:PRO:HB3	1:D:392:THR:OG1	2.14	0.48
1:C:69:PHE:HD2	1:C:74:MET:SD	2.36	0.48
1:B:184:GLN:OE1	1:B:261:ARG:HD2	2.13	0.48
1:A:42:ILE:HD12	4:A:505:GOL:H11	1.93	0.48
1:C:374:VAL:HG12	1:C:376:PHE:N	2.28	0.48
1:A:204:ASN:O	1:A:208:VAL:HG23	2.13	0.48
1:C:387:ILE:N	1:C:387:ILE:HD12	2.29	0.48
1:A:97:ARG:HD3	1:A:367:PRO:O	2.14	0.48
1:A:428:PHE:O	1:A:429:SER:HB3	2.13	0.48
1:D:78:HIS:NE2	1:D:393:SER:HB3	2.28	0.48
1:B:212:TRP:HZ3	1:B:229:THR:HG1	1.61	0.48
1:D:39:ILE:O	1:D:70:GLY:N	2.47	0.48
1:C:370:VAL:HG13	1:C:387:ILE:CD1	2.40	0.48
1:A:365:SER:OG	1:A:366:LEU:N	2.46	0.48
1:B:210:THR:HG22	1:B:212:TRP:H	1.78	0.48
1:D:30:PRO:HG3	1:D:379:TYR:HB3	1.95	0.48
1:D:85:GLU:HA	1:D:89:ASP:OD2	2.13	0.47
1:A:132:ARG:HH22	1:B:321:ALA:HA	1.79	0.47
1:B:79:GLY:O	1:B:83:VAL:HG23	2.13	0.47
1:D:201:LEU:HD11	1:D:296:GLY:HA2	1.95	0.47
1:C:455:ASN:N	1:C:455:ASN:HD22	2.12	0.47
1:D:110:PHE:HA	1:D:119:ARG:HH12	1.76	0.47
1:C:89:ASP:C	1:C:90:LEU:HD12	2.34	0.47
1:D:78:HIS:CD2	1:D:393:SER:HB3	2.49	0.47
1:A:36:LEU:HD22	1:A:39:ILE:HD11	1.95	0.47
1:B:359:ILE:HG13	1:B:360:ASP:N	2.29	0.47
1:D:105:ARG:HH12	1:D:223:ILE:C	2.18	0.47
1:A:355:VAL:O	1:A:359:ILE:HG12	2.13	0.47
1:D:146:GLN:NE2	1:D:338:CYS:HA	2.29	0.47
1:B:436:VAL:HG23	2:B:501:HEM:HBD2	1.97	0.47
1:B:105:ARG:NH1	1:B:234:LEU:HD13	2.30	0.47
1:B:437:GLY:HA3	2:B:501:HEM:HBC2	1.97	0.47
1:D:124:ARG:HH22	1:D:434:ILE:HG22	1.79	0.47
1:A:124:ARG:NH1	1:A:436:VAL:HG23	2.29	0.47
1:C:225:TYR:N	1:C:225:TYR:CD2	2.81	0.47
1:C:185:LYS:HG2	1:C:186:ARG:HG2	1.96	0.47
1:B:105:ARG:HD3	1:B:234:LEU:HD11	1.96	0.47
1:D:247:LYS:HD2	1:D:251:HIS:HE1	1.79	0.47
1:C:97:ARG:NH1	1:C:366:LEU:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:HG12	1:C:376:PHE:H	1.80	0.47
1:C:235:LYS:HE2	1:C:239:PHE:CE2	2.50	0.47
1:B:75:VAL:HB	1:B:387:ILE:CD1	2.44	0.47
1:D:426:MET:N	1:D:427:PRO:CD	2.77	0.47
1:A:333:ARG:NH1	1:A:333:ARG:HG3	2.29	0.47
1:B:394:VAL:HG11	1:B:426:MET:HE3	1.97	0.47
1:D:337:PRO:HD2	1:D:451:PHE:CE1	2.50	0.47
1:D:265:ASP:O	1:D:269:ILE:HG13	2.15	0.47
1:A:394:VAL:HG21	1:A:426:MET:CE	2.45	0.47
1:A:178:ILE:HG22	1:A:182:ILE:HD12	1.96	0.47
1:B:264:ILE:O	1:B:268:LEU:HG	2.15	0.47
1:C:357:ARG:HA	1:C:395:LEU:HD22	1.96	0.47
1:C:442:ARG:HH11	1:C:442:ARG:HG2	1.79	0.47
1:B:205:ILE:HG21	1:B:300:GLU:HG2	1.96	0.47
1:D:425:PHE:C	1:D:427:PRO:HD3	2.35	0.47
1:A:323:VAL:HG12	1:A:327:ILE:HD11	1.96	0.47
1:B:265:ASP:O	1:B:269:ILE:HD13	2.15	0.47
1:B:112:ILE:HD11	1:B:127:SER:OG	2.14	0.47
1:D:251:HIS:HD1	1:D:251:HIS:H	1.63	0.46
1:B:342:ARG:HA	1:B:446:PHE:CZ	2.50	0.46
1:D:35:PRO:HG3	1:D:68:TYR:CD1	2.50	0.46
1:B:183:PHE:HA	1:B:262:ASP:OD2	2.15	0.46
1:A:462:ILE:HD13	1:A:466:ASP:HB2	1.98	0.46
1:B:105:ARG:NH1	1:B:234:LEU:HD22	2.30	0.46
1:A:39:ILE:HB	1:A:42:ILE:CG2	2.45	0.46
1:B:186:ARG:HG2	1:B:187:PHE:H	1.80	0.46
1:B:146:GLN:HG2	1:B:447:LEU:HD13	1.97	0.46
1:D:251:HIS:HA	1:D:261:ARG:NH2	2.29	0.46
1:D:264:ILE:O	1:D:268:LEU:HB2	2.16	0.46
1:A:155:GLU:HG3	1:A:189:TYR:CD1	2.50	0.46
1:B:363:PRO:HD2	1:B:476:PHE:O	2.16	0.46
1:D:101:PRO:HD2	1:D:217:ASN:ND2	2.31	0.46
1:B:394:VAL:HG21	1:B:426:MET:HE3	1.97	0.46
1:D:41:ASN:HA	1:D:44:GLN:OE1	2.15	0.46
1:C:170:LEU:HD13	1:C:307:ARG:HA	1.97	0.46
1:B:39:ILE:HB	1:B:42:ILE:HG22	1.98	0.46
1:C:320:THR:O	1:C:324:GLN:HG3	2.15	0.46
1:B:344:HIS:C	1:B:346:PRO:HD3	2.36	0.46
1:A:83:VAL:HG11	1:A:426:MET:HE1	1.96	0.46
1:A:324:GLN:HA	1:A:327:ILE:HD12	1.98	0.46
1:A:327:ILE:HG12	1:A:345:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:VAL:HA	1:B:335:ARG:NH2	2.31	0.46
1:B:30:PRO:HA	1:B:379:TYR:CD2	2.51	0.46
1:D:57:LEU:HD12	1:D:67:LEU:HD11	1.98	0.46
1:A:408:ASP:HB3	1:A:411:HIS:CE1	2.50	0.46
1:B:394:VAL:HG21	1:B:426:MET:CE	2.46	0.46
1:D:84:LYS:HG2	1:D:88:ILE:HD12	1.98	0.46
1:C:337:PRO:HD3	1:C:454:GLN:OE1	2.15	0.46
1:D:429:SER:HB3	2:D:501:HEM:HBA1	1.98	0.46
1:D:255:MET:HE2	1:D:268:LEU:HD23	1.98	0.46
1:C:318:GLU:HG3	1:C:319:VAL:N	2.30	0.46
1:D:69:PHE:HB3	1:D:218:ASN:OD1	2.15	0.46
1:B:146:GLN:HG2	1:B:447:LEU:CD1	2.45	0.46
1:D:52:LYS:O	1:D:56:ASN:ND2	2.49	0.46
1:A:196:ASN:O	1:A:200:LYS:HB2	2.16	0.46
1:A:420:LYS:HG3	1:A:420:LYS:O	2.16	0.45
1:B:165:ASP:OD2	1:B:166:PRO:HD2	2.16	0.45
1:C:111:GLY:CA	1:C:289:ILE:HG22	2.45	0.45
1:B:75:VAL:HB	1:B:387:ILE:HD13	1.98	0.45
1:A:314:LEU:HD11	1:A:485:LEU:CB	2.46	0.45
1:C:326:GLU:O	1:C:330:VAL:HG23	2.16	0.45
1:A:176:ASN:HD22	1:A:189:TYR:HE2	1.65	0.45
1:D:245:LEU:O	1:D:249:LYS:HG2	2.17	0.45
1:A:31:PRO:HD3	1:A:379:TYR:CE2	2.52	0.45
1:D:85:GLU:O	1:D:89:ASP:HB2	2.17	0.45
1:D:124:ARG:HG3	1:D:128:LEU:CD1	2.47	0.45
1:A:215:ILE:HG12	4:A:505:GOL:H32	1.97	0.45
1:B:441:ALA:HB1	2:B:501:HEM:HAB	1.98	0.45
1:C:362:ILE:HG22	1:C:365:SER:N	2.31	0.45
1:C:102:LEU:HD11	1:C:213:ILE:CG2	2.45	0.45
1:C:97:ARG:NH2	1:C:433:ARG:HD2	2.32	0.45
1:C:318:GLU:HG3	1:C:319:VAL:HG23	1.98	0.45
1:B:56:ASN:O	1:B:59:LYS:HB2	2.17	0.45
1:A:374:VAL:O	1:A:380:LEU:HD12	2.17	0.45
1:B:394:VAL:HG12	1:B:424:TYR:O	2.16	0.45
1:D:170:LEU:HD11	1:D:310:LEU:CD1	2.46	0.45
1:C:321:ALA:O	1:C:325:GLU:HG3	2.17	0.45
1:A:50:VAL:O	1:A:53:SER:HB2	2.17	0.45
1:A:458:LEU:HD22	1:A:485:LEU:CD1	2.47	0.45
1:B:327:ILE:HG12	1:B:345:MET:HE1	1.99	0.45
1:B:365:SER:HB2	1:B:391:LEU:HG	1.99	0.45
1:A:156:LEU:HD22	1:A:487:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:THR:HG22	1:D:212:TRP:H	1.82	0.45
1:C:309:ALA:O	1:C:313:LEU:HG	2.17	0.44
1:B:328:GLU:O	1:B:332:GLY:HA2	2.17	0.44
1:B:207:ILE:O	1:B:213:ILE:HG13	2.17	0.44
1:C:242:SER:O	1:C:246:GLU:HG2	2.17	0.44
1:B:420:LYS:HG3	1:B:420:LYS:O	2.16	0.44
1:C:112:ILE:CD1	1:C:436:VAL:HG21	2.42	0.44
1:A:401:PHE:HB3	1:A:411:HIS:CD2	2.52	0.44
1:C:97:ARG:HB3	1:C:116:ASN:HD21	1.83	0.44
1:D:324:GLN:HA	1:D:327:ILE:CD1	2.42	0.44
1:B:204:ASN:O	1:B:208:VAL:HG23	2.17	0.44
1:B:87:LEU:HD12	1:B:430:ALA:O	2.16	0.44
1:B:124:ARG:NH2	1:B:434:ILE:O	2.50	0.44
1:D:73:ARG:HH21	1:D:382:PRO:HG2	1.82	0.44
1:C:78:HIS:CE1	1:C:393:SER:HB2	2.52	0.44
1:B:285:GLU:O	1:B:289:ILE:HG12	2.18	0.44
1:B:164:CYS:SG	1:B:165:ASP:N	2.90	0.44
1:B:414:ASP:N	1:B:418:ASN:O	2.37	0.44
1:C:205:ILE:HG12	1:C:300:GLU:HG2	1.99	0.44
1:A:29:LEU:HD11	1:A:73:ARG:CZ	2.48	0.44
1:D:261:ARG:HB2	1:D:265:ASP:OD2	2.18	0.44
1:D:372:CYS:HA	1:D:383:LYS:HB2	1.99	0.44
1:C:162:SER:HB3	1:C:163:PRO:HD2	1.99	0.44
1:D:124:ARG:NH2	1:D:434:ILE:HG22	2.33	0.44
1:C:261:ARG:HG3	1:C:261:ARG:NH1	2.33	0.44
1:C:372:CYS:HA	1:C:383:LYS:HB2	2.00	0.44
1:A:470:THR:HA	1:A:471:PRO:HD3	1.89	0.44
1:D:240:MET:O	1:D:244:ILE:HG13	2.17	0.44
1:B:139:ARG:NE	1:B:144:ARG:HG2	2.33	0.44
1:A:107:ASN:O	1:A:108:ARG:HB2	2.18	0.44
1:D:353:HIS:CE1	1:D:419:PHE:HZ	2.36	0.44
1:A:153:VAL:HG13	1:A:456:PHE:CE2	2.53	0.44
1:C:315:LYS:HD3	1:C:467:LEU:O	2.18	0.44
1:B:426:MET:HG2	1:B:430:ALA:HB2	2.00	0.44
1:D:30:PRO:HA	1:D:379:TYR:CD2	2.53	0.44
1:D:128:LEU:HD12	1:D:128:LEU:H	1.83	0.44
1:B:344:HIS:O	1:B:346:PRO:HD3	2.17	0.44
1:A:153:VAL:HG13	1:A:456:PHE:HE2	1.83	0.44
1:A:86:ALA:HB2	1:A:376:PHE:CE1	2.53	0.44
1:A:47:ILE:HA	1:A:47:ILE:HD12	1.89	0.44
1:C:440:LEU:O	1:C:444:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HG21	1:D:345:MET:CG	2.47	0.43
1:A:327:ILE:O	1:A:331:VAL:HB	2.18	0.43
1:B:136:MET:SD	1:B:181:ILE:HG23	2.57	0.43
1:D:365:SER:OG	1:D:366:LEU:N	2.49	0.43
1:C:70:GLY:O	1:C:71:LEU:HB3	2.18	0.43
1:C:330:VAL:HG11	1:C:344:HIS:HB2	2.00	0.43
1:C:319:VAL:O	1:C:323:VAL:HG23	2.17	0.43
1:B:414:ASP:HB3	1:B:418:ASN:H	1.83	0.43
1:B:246:GLU:O	1:B:250:GLU:HG3	2.18	0.43
1:A:454:GLN:O	1:A:454:GLN:HG2	2.19	0.43
1:B:129:MET:O	1:B:132:ARG:HG3	2.17	0.43
1:C:119:ARG:HG2	1:C:281:GLU:CD	2.39	0.43
1:B:52:LYS:HD3	1:B:52:LYS:O	2.19	0.43
1:C:104:GLU:O	1:C:108:ARG:HA	2.18	0.43
1:A:331:VAL:HA	1:A:335:ARG:NH2	2.34	0.43
1:C:229:THR:O	1:C:232:LYS:HB3	2.17	0.43
1:C:488:ILE:N	1:C:488:ILE:HD12	2.33	0.43
1:C:308:TYR:OH	1:C:471:PRO:HG3	2.18	0.43
1:D:251:HIS:O	1:D:255:MET:HB2	2.18	0.43
1:A:429:SER:CB	2:A:501:HEM:HBA1	2.49	0.43
1:D:205:ILE:HG13	1:D:300:GLU:CG	2.49	0.43
1:C:30:PRO:HA	1:C:379:TYR:CD2	2.53	0.43
1:B:283:THR:CG2	1:B:286:ASN:HB2	2.48	0.43
1:A:223:ILE:CD1	1:A:230:HIS:ND1	2.82	0.43
1:D:376:PHE:CD2	1:D:377:ARG:HG3	2.54	0.43
1:C:366:LEU:HG	3:C:502:OXV:H2	2.01	0.43
1:D:414:ASP:OD2	1:D:418:ASN:HB2	2.19	0.43
1:D:218:ASN:O	1:D:220:PRO:HD3	2.19	0.43
1:A:432:LYS:HB3	1:A:432:LYS:HE3	1.79	0.43
1:B:154:GLU:O	1:B:158:LYS:HG2	2.18	0.43
1:B:311:LEU:HB2	1:B:483:TYR:CE2	2.54	0.43
1:C:145:VAL:HG11	1:C:447:LEU:HD12	2.01	0.43
1:C:267:PHE:CD2	1:C:287:LEU:HD22	2.52	0.43
1:C:360:ASP:OD2	1:C:392:THR:HB	2.19	0.43
1:A:440:LEU:O	1:A:444:GLU:HG3	2.19	0.43
1:D:111:GLY:CA	1:D:289:ILE:HG22	2.49	0.43
1:B:235:LYS:O	1:B:239:PHE:HD1	2.02	0.43
1:D:93:GLU:O	1:D:370:VAL:HA	2.18	0.43
1:C:272:GLU:HA	1:C:275:LYS:HB2	2.01	0.42
1:B:433:ARG:HB3	2:B:501:HEM:O2A	2.18	0.42
1:D:238:ALA:O	1:D:241:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASP:HB3	1:C:259:ASN:HB3	1.99	0.42
1:B:354:GLU:HA	1:B:354:GLU:OE1	2.19	0.42
1:A:314:LEU:HD11	1:A:485:LEU:HB3	1.99	0.42
1:A:72:GLU:HG2	5:A:614:HOH:O	2.19	0.42
1:A:401:PHE:O	1:A:404:PRO:HD3	2.18	0.42
1:C:31:PRO:HD3	1:C:379:TYR:CE2	2.54	0.42
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.83	0.42
1:B:49:ASP:HA	1:B:473:VAL:HG11	2.02	0.42
1:B:355:VAL:O	1:B:359:ILE:HG23	2.19	0.42
1:B:105:ARG:CZ	1:B:234:LEU:HD13	2.49	0.42
1:C:36:LEU:HD12	1:C:43:LEU:HD12	2.01	0.42
1:A:90:LEU:HB3	1:A:93:GLU:HG3	2.01	0.42
1:D:113:VAL:HG22	2:D:501:HEM:HAD1	2.01	0.42
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.84	0.42
1:C:105:ARG:HE	1:C:234:LEU:CD1	2.31	0.42
1:D:346:PRO:HG2	1:D:347:TYR:H	1.83	0.42
1:B:368:HIS:NE2	1:B:433:ARG:CB	2.82	0.42
1:C:85:GLU:O	1:C:89:ASP:HB2	2.20	0.42
1:A:149:ALA:O	1:A:153:VAL:HG23	2.20	0.42
1:D:83:VAL:HG13	1:D:87:LEU:HD23	2.01	0.42
1:C:307:ARG:NH1	5:C:612:HOH:O	2.47	0.42
1:D:38:VAL:HG12	1:D:39:ILE:N	2.35	0.42
1:B:267:PHE:CD2	1:B:287:LEU:HB2	2.55	0.42
1:A:42:ILE:HG23	1:A:43:LEU:N	2.32	0.42
1:C:425:PHE:C	1:C:427:PRO:HD3	2.40	0.42
1:B:139:ARG:HD3	1:B:144:ARG:NH1	2.34	0.42
1:C:330:VAL:O	1:C:330:VAL:HG12	2.19	0.42
1:A:178:ILE:HG21	1:A:295:LEU:HA	2.02	0.42
1:D:412:PHE:HB3	1:D:419:PHE:HE2	1.85	0.42
1:C:85:GLU:O	1:C:90:LEU:HD13	2.20	0.42
1:D:30:PRO:HG3	1:D:379:TYR:CB	2.50	0.42
1:A:152:LEU:O	1:A:156:LEU:HG	2.20	0.42
1:B:463:ASP:OD2	1:B:465:LYS:HD2	2.19	0.42
1:A:84:LYS:CG	1:A:88:ILE:HD12	2.26	0.42
1:D:445:LEU:O	1:D:449:LEU:HD12	2.20	0.42
1:B:320:THR:O	1:B:324:GLN:HG3	2.19	0.42
1:C:426:MET:N	1:C:427:PRO:CD	2.82	0.42
1:B:275:LYS:HG2	1:B:276:GLN:HG3	2.01	0.42
1:C:212:TRP:O	1:C:215:ILE:HG22	2.20	0.42
1:B:308:TYR:OH	1:B:471:PRO:HG3	2.20	0.42
1:A:173:ALA:HB3	1:A:174:PRO:CD	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:O	1:D:119:ARG:C	2.58	0.41
1:B:156:LEU:O	1:B:159:THR:HG22	2.20	0.41
1:C:428:PHE:O	1:C:429:SER:HB3	2.20	0.41
1:B:86:ALA:HB2	1:B:376:PHE:CE1	2.54	0.41
1:D:436:VAL:HG23	2:D:501:HEM:HBD2	2.02	0.41
1:B:339:MET:O	1:B:342:ARG:HB3	2.20	0.41
1:C:403:ASN:HB3	1:C:406:MET:HG3	2.00	0.41
1:B:49:ASP:CG	1:B:52:LYS:HB2	2.41	0.41
1:B:123:ILE:HG13	1:B:286:ASN:ND2	2.35	0.41
1:B:365:SER:HB2	1:B:391:LEU:CG	2.51	0.41
1:C:455:ASN:O	1:C:489:PRO:HA	2.20	0.41
1:B:182:ILE:HG22	1:B:183:PHE:CE1	2.55	0.41
1:A:184:GLN:HG3	1:A:185:LYS:HG2	2.01	0.41
1:A:252:GLN:HG2	1:A:268:LEU:CD2	2.50	0.41
1:C:370:VAL:HG21	1:C:381:ILE:HG22	2.01	0.41
1:C:377:ARG:O	1:C:378:ASN:C	2.58	0.41
1:A:444:GLU:HB3	1:A:448:PHE:CE2	2.55	0.41
1:D:204:ASN:O	1:D:208:VAL:HG23	2.20	0.41
1:C:35:PRO:HB2	1:C:40:GLY:HA2	2.02	0.41
1:B:370:VAL:HG23	1:B:370:VAL:O	2.20	0.41
1:D:471:PRO:HB2	1:D:473:VAL:HG13	2.03	0.41
1:B:49:ASP:HA	1:B:473:VAL:CG1	2.51	0.41
1:A:252:GLN:HG2	1:A:268:LEU:HD21	2.03	0.41
1:C:311:LEU:HB2	1:C:483:TYR:CE2	2.55	0.41
1:C:181:ILE:O	1:C:263:PHE:HB2	2.21	0.41
1:A:223:ILE:O	1:A:223:ILE:HD12	2.21	0.41
1:B:187:PHE:CG	1:B:194:PHE:HB2	2.55	0.41
1:A:426:MET:N	1:A:427:PRO:CD	2.84	0.41
1:D:86:ALA:HB2	1:D:376:PHE:CE1	2.55	0.41
1:A:178:ILE:HG22	1:A:182:ILE:CD1	2.51	0.41
1:C:382:PRO:HG2	1:C:385:THR:OG1	2.20	0.41
1:A:173:ALA:O	1:A:177:VAL:HG23	2.19	0.41
1:B:110:PHE:HB2	1:B:289:ILE:HG13	2.03	0.41
1:C:39:ILE:HB	1:C:42:ILE:CG1	2.49	0.41
1:D:444:GLU:O	1:D:448:PHE:HB2	2.20	0.41
1:A:148:GLU:OE2	1:A:176:ASN:HB3	2.21	0.41
1:B:430:ALA:HA	1:B:434:ILE:HD12	2.01	0.41
1:C:85:GLU:CD	1:C:377:ARG:HH21	2.24	0.41
1:D:51:SER:OG	1:D:363:PRO:HB3	2.20	0.41
1:C:318:GLU:CG	1:C:319:VAL:N	2.84	0.41
1:B:278:GLN:HG3	1:B:279:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:VAL:HG13	1:B:480:PRO:HD2	2.02	0.41
1:D:488:ILE:N	1:D:488:ILE:HD12	2.36	0.41
1:C:38:VAL:HG12	1:C:38:VAL:O	2.21	0.41
1:A:400:GLU:HG2	1:A:424:TYR:CG	2.56	0.41
1:D:153:VAL:HG13	1:D:455:ASN:HD21	1.86	0.41
1:A:42:ILE:CG2	1:A:43:LEU:N	2.84	0.41
1:C:36:LEU:HD23	1:C:36:LEU:HA	1.94	0.41
1:B:230:HIS:O	1:B:233:LEU:HB3	2.21	0.41
1:D:102:LEU:HB2	1:D:217:ASN:OD1	2.21	0.41
1:D:101:PRO:O	1:D:104:GLU:HB3	2.21	0.41
1:B:124:ARG:NH1	1:B:433:ARG:HA	2.36	0.41
1:A:205:ILE:HA	1:A:205:ILE:HD12	1.72	0.41
1:C:225:TYR:HD2	1:C:225:TYR:N	2.19	0.41
1:C:428:PHE:CG	1:C:438:GLU:HG2	2.56	0.41
1:B:97:ARG:HD3	1:B:367:PRO:O	2.21	0.41
1:D:65:PHE:CE1	1:D:76:VAL:HB	2.56	0.41
1:C:219:PHE:O	1:C:222:ILE:HG22	2.21	0.41
1:B:173:ALA:CB	1:B:174:PRO:HD3	2.41	0.41
1:A:368:HIS:HE1	1:A:433:ARG:HB2	1.86	0.41
1:D:405:GLU:HG2	1:D:406:MET:N	2.36	0.41
1:D:357:ARG:HD2	1:D:401:PHE:CD1	2.56	0.41
1:A:463:ASP:OD2	1:A:465:LYS:HB2	2.21	0.40
1:B:257:ILE:O	1:B:257:ILE:HG22	2.20	0.40
1:A:213:ILE:HA	1:A:213:ILE:HD13	1.92	0.40
1:C:30:PRO:HA	1:C:379:TYR:CG	2.56	0.40
1:C:120:TRP:CZ2	1:C:124:ARG:HD2	2.56	0.40
1:C:400:GLU:HG2	1:C:424:TYR:HB2	2.04	0.40
1:B:54:LEU:O	1:B:57:LEU:HB2	2.21	0.40
1:D:39:ILE:HG13	1:D:40:GLY:N	2.36	0.40
1:B:110:PHE:N	1:B:110:PHE:CD1	2.89	0.40
1:D:148:GLU:OE1	1:D:173:ALA:HA	2.21	0.40
1:C:182:ILE:HA	1:C:263:PHE:CB	2.51	0.40
1:C:69:PHE:HB2	1:C:74:MET:CE	2.51	0.40
1:B:225:TYR:CG	1:B:226:PHE:N	2.89	0.40
1:D:248:VAL:HA	1:D:264:ILE:HG21	2.03	0.40
1:A:376:PHE:O	1:A:377:ARG:HD3	2.22	0.40
1:A:275:LYS:HG2	1:A:275:LYS:O	2.21	0.40
1:C:354:GLU:HA	1:C:354:GLU:OE2	2.21	0.40
1:A:311:LEU:HB2	1:A:483:TYR:CE2	2.56	0.40
1:A:463:ASP:OD1	1:A:464:PRO:HD2	2.20	0.40
1:B:184:GLN:HG3	1:B:185:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:THR:O	1:C:160:LYS:HB2	2.21	0.40
1:C:327:ILE:HA	1:C:345:MET:HE1	2.04	0.40
1:B:326:GLU:HG2	1:B:345:MET:HE2	2.04	0.40
1:C:86:ALA:HB1	1:C:94:PHE:CZ	2.57	0.40
1:D:359:ILE:HG13	1:D:360:ASP:N	2.35	0.40
1:D:374:VAL:HG12	1:D:375:LYS:N	2.35	0.40
1:A:459:LYS:HB3	1:A:488:ILE:CD1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/477 (97%)	418 (90%)	42 (9%)	2 (0%)	39	73
1	B	452/477 (95%)	411 (91%)	34 (8%)	7 (2%)	13	40
1	C	460/477 (96%)	415 (90%)	43 (9%)	2 (0%)	39	73
1	D	448/477 (94%)	396 (88%)	51 (11%)	1 (0%)	52	83
All	All	1822/1908 (96%)	1640 (90%)	170 (9%)	12 (1%)	26	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	GLY
1	B	365	SER
1	A	429	SER
1	D	31	PRO
1	B	429	SER
1	C	228	GLY
1	B	91	GLY
1	B	215	ILE

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Mol	Chain	Res	Type
1	B	227	PRO
1	C	31	PRO
1	A	47	ILE
1	B	101	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	421/431 (98%)	418 (99%)	3 (1%)	88	96
1	B	413/431 (96%)	407 (98%)	6 (2%)	72	91
1	C	417/431 (97%)	411 (99%)	6 (1%)	74	92
1	D	405/431 (94%)	400 (99%)	5 (1%)	78	93
All	All	1656/1724 (96%)	1636 (99%)	20 (1%)	78	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PHE
1	A	219	PHE
1	A	308	TYR
1	B	99	HIS
1	B	176	ASN
1	B	308	TYR
1	B	362	ILE
1	B	368	HIS
1	B	379	TYR
1	C	87	LEU
1	C	100	PHE
1	C	216	CYS
1	C	265	ASP
1	C	308	TYR
1	C	379	TYR
1	D	99	HIS
1	D	302	THR

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Mol	Chain	Res	Type
1	D	308	TYR
1	D	318	GLU
1	D	362	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	457	ASN
1	A	474	ASN
1	B	146	GLN
1	B	231	ASN
1	B	236	ASN
1	C	196	ASN
1	C	214	GLN
1	C	218	ASN
1	C	378	ASN
1	D	56	ASN
1	D	176	ASN
1	D	192	GLN
1	D	214	GLN
1	D	231	ASN
1	D	277	ASN
1	D	403	ASN
1	D	454	GLN
1	D	455	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

11 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	501	1,5	30,50,50	3.73	14 (46%)	24,82,82	2.69	10 (41%)
3	0XV	A	502	-	18,23,23	2.26	9 (50%)	23,34,34	1.41	4 (17%)
4	GOL	A	503	-	5,5,5	0.24	0	5,5,5	0.21	0
4	GOL	A	504	-	5,5,5	0.29	0	5,5,5	0.24	0
4	GOL	A	505	-	5,5,5	0.26	0	5,5,5	0.23	0
2	HEM	B	501	1	30,50,50	3.76	14 (46%)	24,82,82	2.68	10 (41%)
3	0XV	B	502	-	18,23,23	2.27	10 (55%)	23,34,34	1.37	4 (17%)
2	HEM	C	501	1	30,50,50	3.80	14 (46%)	24,82,82	2.69	10 (41%)
3	0XV	C	502	-	18,23,23	2.31	10 (55%)	23,34,34	1.41	4 (17%)
2	HEM	D	501	1	30,50,50	3.75	14 (46%)	24,82,82	2.65	11 (45%)
3	0XV	D	502	-	18,23,23	2.29	10 (55%)	23,34,34	1.40	4 (17%)

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	501	1,5	-	0/10/54/54	0/0/8/8
3	0XV	A	502	-	-	0/5/8/8	0/2/3/3
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
4	GOL	A	504	-	-	0/4/4/4	0/0/0/0
4	GOL	A	505	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	0XV	B	502	-	-	0/5/8/8	0/2/3/3
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
3	0XV	C	502	-	-	0/5/8/8	0/2/3/3
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	0XV	D	502	-	-	0/5/8/8	0/2/3/3



All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3B-C4B	-10.73	1.42	1.51
2	B	501	HEM	C3B-C4B	-10.49	1.42	1.51
2	D	501	HEM	C3B-C4B	-10.36	1.42	1.51
2	A	501	HEM	C3B-C4B	-10.27	1.42	1.51
2	B	501	HEM	C3D-C4D	-8.03	1.41	1.51
2	A	501	HEM	C3D-C4D	-7.93	1.41	1.51
2	D	501	HEM	C3D-C4D	-7.93	1.41	1.51
2	C	501	HEM	C3D-C4D	-7.89	1.41	1.51
2	C	501	HEM	C2C-C1C	-7.55	1.38	1.52
2	A	501	HEM	C2C-C1C	-7.44	1.38	1.52
2	B	501	HEM	C2C-C1C	-7.43	1.38	1.52
2	D	501	HEM	C2C-C1C	-7.42	1.38	1.52
2	A	501	HEM	C3C-CAC	-7.35	1.37	1.51
2	B	501	HEM	C3C-CAC	-7.35	1.37	1.51
2	D	501	HEM	C3C-CAC	-7.34	1.37	1.51
2	C	501	HEM	C3C-CAC	-7.31	1.37	1.51
2	D	501	HEM	C2D-C3D	-5.84	1.37	1.54
2	B	501	HEM	C2D-C3D	-5.80	1.37	1.54
2	A	501	HEM	C2D-C3D	-5.76	1.37	1.54
2	C	501	HEM	C2D-C3D	-5.74	1.37	1.54
2	D	501	HEM	C3B-CAB	-4.79	1.42	1.51
2	C	501	HEM	C3B-CAB	-4.68	1.42	1.51
2	B	501	HEM	C3B-CAB	-4.63	1.42	1.51
2	A	501	HEM	C3B-CAB	-4.53	1.42	1.51
2	D	501	HEM	C2D-C1D	-3.52	1.40	1.51
2	C	501	HEM	C2D-C1D	-3.44	1.40	1.51
2	A	501	HEM	C2D-C1D	-3.40	1.40	1.51
2	B	501	HEM	C2D-C1D	-3.37	1.40	1.51
2	B	501	HEM	C1C-NC	-3.13	1.32	1.36
2	C	501	HEM	C1C-NC	-3.01	1.32	1.36
2	A	501	HEM	C1C-NC	-3.00	1.32	1.36
2	D	501	HEM	C1C-NC	-2.94	1.32	1.36
2	A	501	HEM	C2B-C1B	-2.85	1.42	1.51
2	B	501	HEM	C2B-C1B	-2.85	1.42	1.51
2	C	501	HEM	C2B-C1B	-2.82	1.42	1.51
2	D	501	HEM	C2B-C1B	-2.80	1.42	1.51
3	D	502	0XV	CAC-CAB	2.02	1.42	1.38
3	D	502	0XV	CAP-CAQ	2.04	1.42	1.40
3	B	502	0XV	CAC-CAB	2.04	1.42	1.38
3	B	502	0XV	CAP-CAQ	2.06	1.42	1.40
3	A	502	0XV	CAC-CAB	2.07	1.42	1.38
3	C	502	0XV	CAC-CAB	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	0XV	CAP-CAQ	2.11	1.42	1.40
3	D	502	0XV	CAP-CAN	2.17	1.42	1.40
3	B	502	0XV	CAP-CAN	2.19	1.43	1.40
3	C	502	0XV	CAM-CAL	2.20	1.42	1.39
3	A	502	0XV	CAP-CAN	2.20	1.43	1.40
2	A	501	HEM	FE-NB	2.20	2.09	1.97
3	C	502	0XV	CAP-CAN	2.22	1.43	1.40
2	B	501	HEM	FE-ND	2.24	2.09	1.97
3	A	502	0XV	CAM-CAL	2.26	1.42	1.39
2	B	501	HEM	CBC-CAC	2.26	1.42	1.29
3	B	502	0XV	CAM-CAL	2.26	1.42	1.39
2	D	501	HEM	CBC-CAC	2.27	1.42	1.29
2	A	501	HEM	CBC-CAC	2.27	1.42	1.29
3	A	502	0XV	CAD-CAC	2.28	1.41	1.36
2	C	501	HEM	CBC-CAC	2.29	1.42	1.29
2	D	501	HEM	FE-ND	2.31	2.09	1.97
3	D	502	0XV	CAM-CAL	2.32	1.42	1.39
3	A	502	0XV	CAE-CAF	2.35	1.42	1.36
2	B	501	HEM	FE-NC	2.38	2.05	1.95
2	A	501	HEM	FE-NC	2.43	2.05	1.95
3	B	502	0XV	CAD-CAC	2.45	1.42	1.36
3	C	502	0XV	CAE-CAF	2.45	1.42	1.36
3	B	502	0XV	CAE-CAF	2.47	1.42	1.36
3	D	502	0XV	CAD-CAC	2.47	1.42	1.36
3	C	502	0XV	CAD-CAC	2.48	1.42	1.36
3	D	502	0XV	CAU-CAL	2.49	1.43	1.39
3	B	502	0XV	CAU-CAL	2.51	1.43	1.39
3	D	502	0XV	CAE-CAF	2.52	1.42	1.36
3	A	502	0XV	CAU-CAL	2.54	1.43	1.39
3	C	502	0XV	CAU-CAL	2.58	1.43	1.39
2	D	501	HEM	FE-NC	2.75	2.06	1.95
2	C	501	HEM	FE-ND	2.76	2.12	1.97
2	C	501	HEM	FE-NC	2.98	2.07	1.95
3	B	502	0XV	CAV-CAI	3.04	1.53	1.48
3	A	502	0XV	CAV-CAI	3.07	1.53	1.48
2	A	501	HEM	CMA-C3A	3.14	1.58	1.51
2	D	501	HEM	CMA-C3A	3.16	1.58	1.51
2	C	501	HEM	CMA-C3A	3.18	1.58	1.51
2	B	501	HEM	CMA-C3A	3.22	1.58	1.51
3	D	502	0XV	CAV-CAI	3.22	1.53	1.48
3	C	502	0XV	CAV-CAI	3.31	1.53	1.48
2	B	501	HEM	CBB-CAB	3.32	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CBB-CAB	3.32	1.48	1.29
2	D	501	HEM	CBB-CAB	3.35	1.48	1.29
2	A	501	HEM	CBB-CAB	3.38	1.48	1.29
3	B	502	0XV	CAL-CAJ	3.95	1.56	1.49
3	D	502	0XV	CAL-CAJ	4.02	1.56	1.49
3	A	502	0XV	CAL-CAJ	4.04	1.56	1.49
3	C	502	0XV	CAL-CAJ	4.07	1.56	1.49
3	D	502	0XV	CAG-CAJ	4.16	1.55	1.50
3	C	502	0XV	CAG-CAJ	4.17	1.55	1.50
3	B	502	0XV	CAG-CAJ	4.17	1.55	1.50
3	A	502	0XV	CAG-CAJ	4.25	1.55	1.50

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	0XV	CAQ-CAP-CAN	-3.60	118.92	121.64
3	A	502	0XV	CAQ-CAP-CAN	-3.54	118.96	121.64
3	D	502	0XV	CAQ-CAP-CAN	-3.51	118.98	121.64
3	B	502	0XV	CAQ-CAP-CAN	-3.50	118.99	121.64
2	D	501	HEM	C3B-C4B-CHC	2.01	125.99	123.16
3	B	502	0XV	CAG-CAJ-CAL	2.32	122.95	119.55
2	A	501	HEM	CBA-CAA-C2A	2.40	116.83	112.53
2	D	501	HEM	CBA-CAA-C2A	2.41	116.85	112.53
2	C	501	HEM	CBA-CAA-C2A	2.46	116.94	112.53
3	C	502	0XV	CAG-CAJ-CAL	2.47	123.17	119.55
2	B	501	HEM	CBA-CAA-C2A	2.47	116.95	112.53
3	A	502	0XV	CAG-CAJ-CAL	2.48	123.19	119.55
3	D	502	0XV	CAG-CAJ-CAL	2.51	123.23	119.55
2	D	501	HEM	CMD-C2D-C3D	2.53	125.53	114.35
2	B	501	HEM	CMD-C2D-C3D	2.53	125.55	114.35
2	A	501	HEM	CMD-C2D-C3D	2.54	125.59	114.35
2	C	501	HEM	CMD-C2D-C3D	2.55	125.64	114.35
2	D	501	HEM	C1D-CHD-C4C	2.72	130.37	125.82
2	B	501	HEM	C1D-CHD-C4C	2.75	130.41	125.82
3	B	502	0XV	CAU-CAQ-CAP	2.78	120.40	118.08
3	C	502	0XV	CAU-CAQ-CAP	2.81	120.43	118.08
2	A	501	HEM	C1D-CHD-C4C	2.82	130.53	125.82
3	D	502	0XV	CAU-CAQ-CAP	2.83	120.44	118.08
3	A	502	0XV	CAU-CAQ-CAP	2.85	120.46	118.08
2	C	501	HEM	C1D-CHD-C4C	3.00	130.84	125.82
3	B	502	0XV	CAM-CAN-CAP	3.11	120.68	118.08
3	D	502	0XV	CAM-CAN-CAP	3.11	120.68	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	0XV	CAM-CAN-CAP	3.15	120.71	118.08
3	C	502	0XV	CAM-CAN-CAP	3.17	120.73	118.08
2	C	501	HEM	C3C-CAC-CBC	3.29	129.50	124.46
2	D	501	HEM	C3C-CAC-CBC	3.38	129.63	124.46
2	B	501	HEM	C4B-CHC-C1C	3.39	131.48	125.82
2	A	501	HEM	C3C-CAC-CBC	3.41	129.68	124.46
2	D	501	HEM	C4B-CHC-C1C	3.45	131.59	125.82
2	B	501	HEM	C3C-CAC-CBC	3.45	129.75	124.46
2	A	501	HEM	C4B-CHC-C1C	3.47	131.62	125.82
2	D	501	HEM	C3B-CAB-CBB	3.61	130.00	124.46
2	C	501	HEM	C4B-CHC-C1C	3.66	131.95	125.82
2	B	501	HEM	C3B-CAB-CBB	3.93	130.49	124.46
2	A	501	HEM	C3B-CAB-CBB	4.00	130.59	124.46
2	C	501	HEM	C3B-CAB-CBB	4.02	130.62	124.46
2	B	501	HEM	CAD-C3D-C4D	4.32	127.72	112.47
2	A	501	HEM	CAD-C3D-C4D	4.32	127.72	112.47
2	C	501	HEM	CAD-C3D-C4D	4.36	127.84	112.47
2	D	501	HEM	CMC-C2C-C3C	4.38	127.45	116.53
2	C	501	HEM	CMC-C2C-C3C	4.40	127.51	116.53
2	B	501	HEM	CMC-C2C-C3C	4.43	127.58	116.53
2	A	501	HEM	CMC-C2C-C3C	4.43	127.58	116.53
2	D	501	HEM	CAD-C3D-C4D	4.46	128.21	112.47
2	D	501	HEM	CAD-C3D-C2D	5.08	127.83	113.22
2	C	501	HEM	CAD-C3D-C2D	5.21	128.20	113.22
2	B	501	HEM	CAD-C3D-C2D	5.25	128.31	113.22
2	A	501	HEM	CAD-C3D-C2D	5.26	128.34	113.22
2	D	501	HEM	CMB-C2B-C3B	5.35	129.88	116.53
2	C	501	HEM	CMB-C2B-C3B	5.45	130.12	116.53
2	A	501	HEM	CMB-C2B-C3B	5.46	130.15	116.53
2	B	501	HEM	CMB-C2B-C3B	5.47	130.18	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
3	A	502	0XV	1	0
4	A	505	GOL	3	0
2	B	501	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	0XV	2	0
3	C	502	0XV	1	0
2	D	501	HEM	3	0
3	D	502	0XV	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	464/477 (97%)	0.11	2 (0%) 93 92	47, 68, 92, 113	0
1	B	456/477 (95%)	0.36	10 (2%) 65 62	55, 87, 117, 125	0
1	C	462/477 (96%)	0.23	9 (1%) 70 67	57, 86, 107, 127	0
1	D	452/477 (94%)	0.43	22 (4%) 33 28	65, 102, 128, 133	0
All	All	1834/1908 (96%)	0.28	43 (2%) 64 60	47, 85, 119, 133	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	GLN	3.9
1	D	473	VAL	3.7
1	D	214	GLN	3.4
1	D	260	PRO	3.3
1	C	458	LEU	3.2
1	D	476	PHE	2.9
1	D	487	PHE	2.9
1	C	476	PHE	2.9
1	C	225	TYR	2.8
1	B	164	CYS	2.8
1	A	216	CYS	2.6
1	C	212	TRP	2.6
1	C	257	ILE	2.5
1	D	265	ASP	2.5
1	D	123	ILE	2.5
1	D	194	PHE	2.4
1	D	45	ILE	2.4
1	D	215	ILE	2.4
1	D	244	ILE	2.4
1	D	248	VAL	2.4
1	B	276	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	193	GLN	2.3
1	B	248	VAL	2.3
1	B	331	VAL	2.3
1	C	314	LEU	2.3
1	D	268	LEU	2.3
1	D	468	ASP	2.2
1	C	207	ILE	2.2
1	B	39	ILE	2.2
1	D	240	MET	2.2
1	D	187	PHE	2.1
1	D	334	ASN	2.1
1	B	187	PHE	2.1
1	B	436	VAL	2.1
1	D	287	LEU	2.1
1	D	330	VAL	2.1
1	A	230	HIS	2.1
1	B	263	PHE	2.1
1	D	331	VAL	2.1
1	B	136	MET	2.0
1	C	453	LEU	2.0
1	D	458	LEU	2.0
1	C	311	LEU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	0XV	C	502	21/21	0.90	0.39	2.12	78,81,83,83	0
3	0XV	B	502	21/21	0.88	0.34	1.96	77,84,86,87	0
3	0XV	A	502	21/21	0.95	0.28	1.65	52,54,58,58	0
2	HEM	D	501	43/43	0.97	0.34	1.61	91,95,98,99	0
3	0XV	D	502	21/21	0.88	0.34	1.20	95,97,99,99	0
2	HEM	B	501	43/43	0.97	0.28	0.82	77,80,88,90	0
2	HEM	C	501	43/43	0.98	0.22	-0.18	55,59,61,66	0
2	HEM	A	501	43/43	0.98	0.19	-0.66	37,44,54,57	0
4	GOL	A	503	6/6	0.89	0.18	-0.98	68,70,71,72	0
4	GOL	A	505	6/6	0.87	0.18	-0.99	89,90,90,90	0
4	GOL	A	504	6/6	0.87	0.17	-	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.