



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:32 AM GMT

PDB ID : 3IR5  
Title : Crystal structure of NarGHI mutant NarG-H49C  
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.  
Deposited on : 2009-08-21  
Resolution : 2.30 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

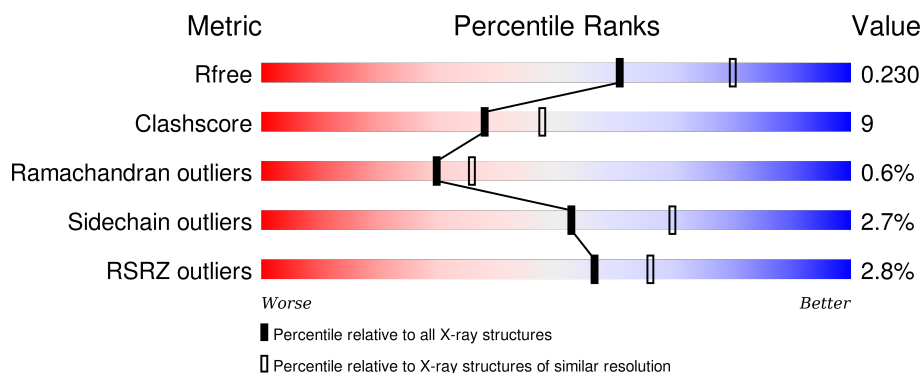
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	1247	<div> <div>4%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
2	B	512	<div> <div>83%</div> <div>16%</div> <div>..</div> </div>
3	C	225	<div> <div>5%</div> <div>75%</div> <div>22%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	B	803	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16376 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 Respiratory nitrate reductase 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0	0
			9865	6229	1729	1858	49			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	CYS	HIS	ENGINEERED	UNP P09152

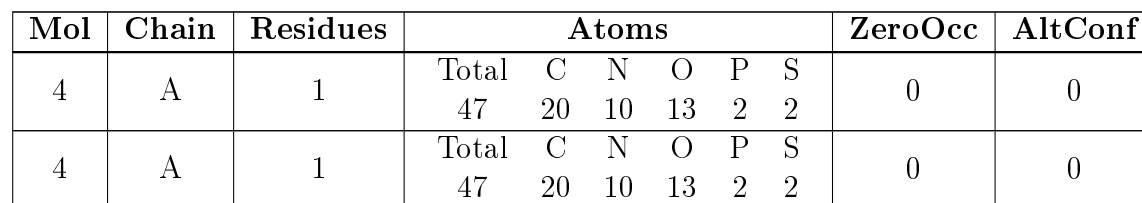
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	509	Total	C	N	O	S	0	0	0
			4050	2562	701	755	32			

- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1747	1158	295	281	13			

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).

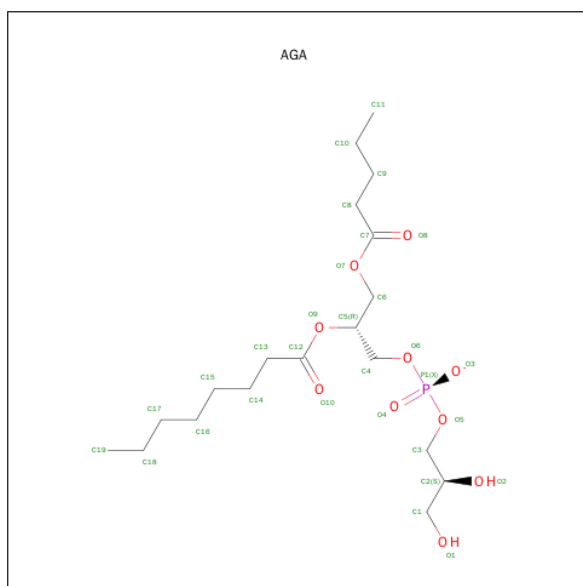


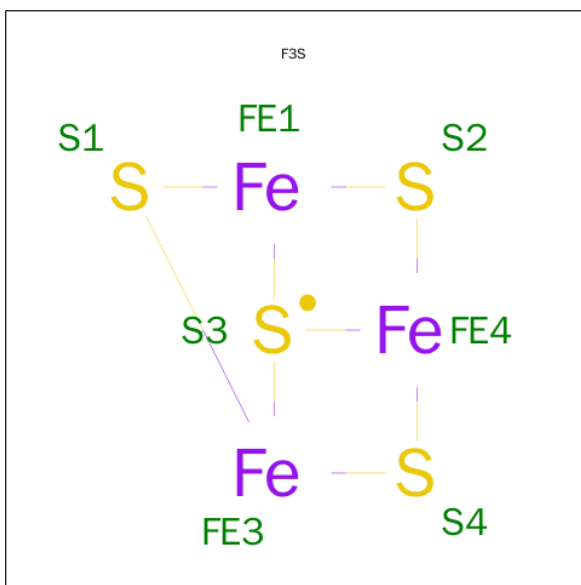
- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | A     | 1        | Total Mo<br>1 1 | 0       | 0       |

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

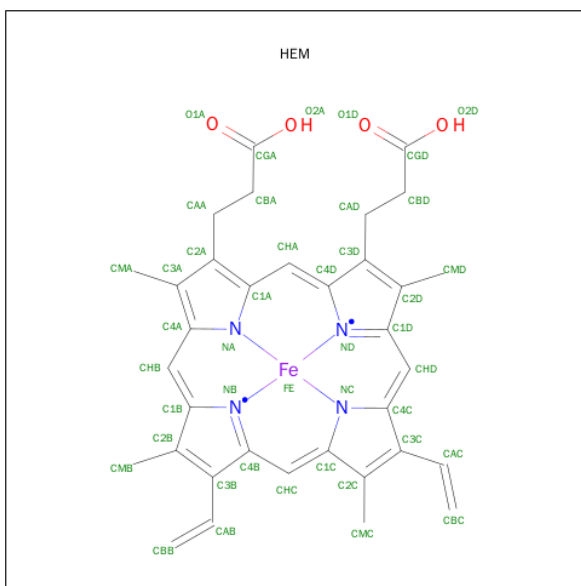
- Molecule 7 is (1S)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: C<sub>19</sub>H<sub>36</sub>O<sub>10</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	Fe	S		0	0
			7	3	4			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 10 is water.

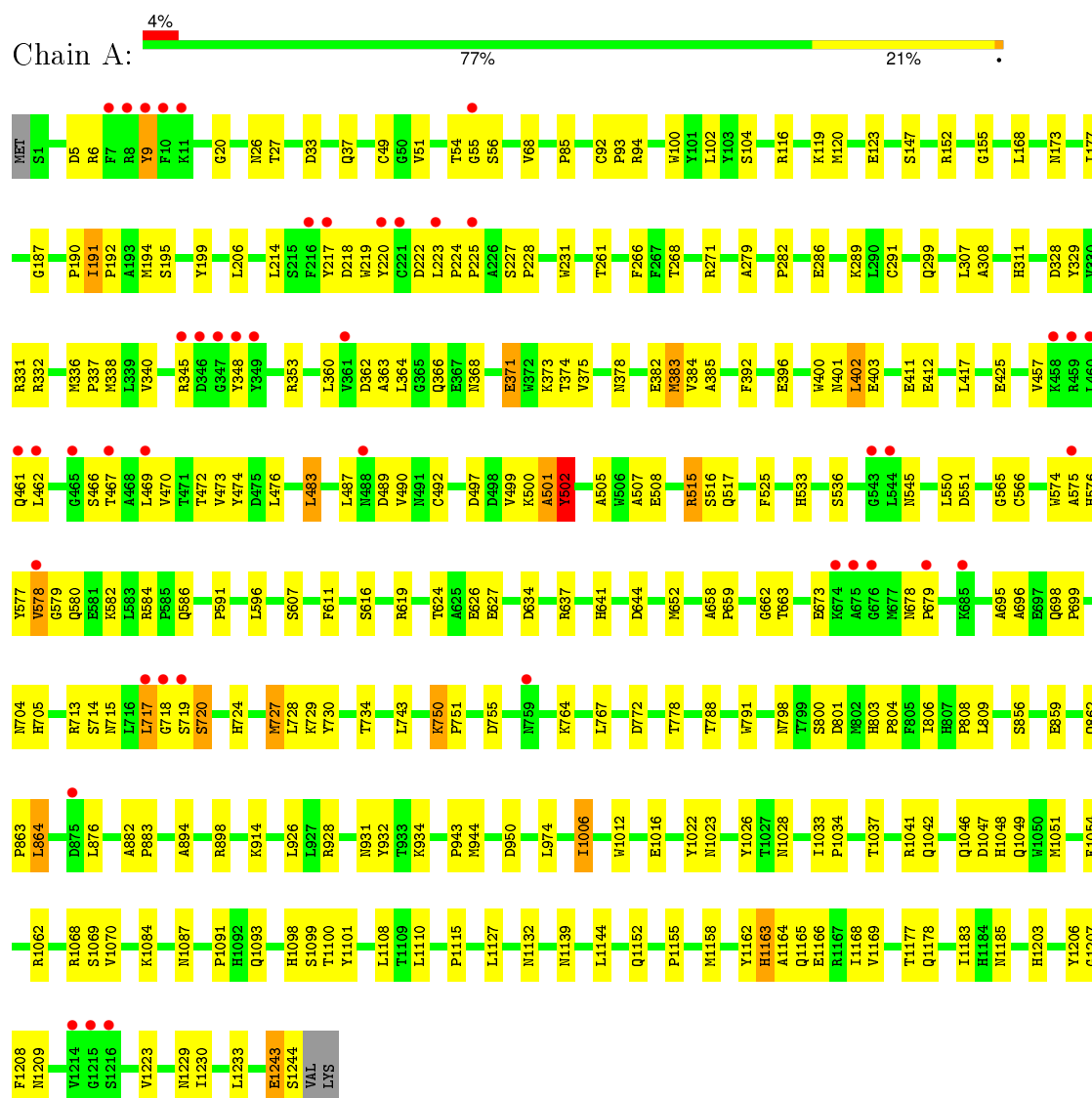
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	253	Total 253	O 253	0	0
10	B	182	Total 182	O 182	0	0
10	C	34	Total 34	O 34	0	0



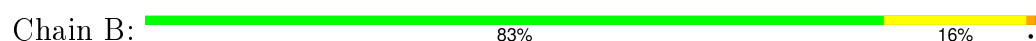
### 3 Residue-property plots

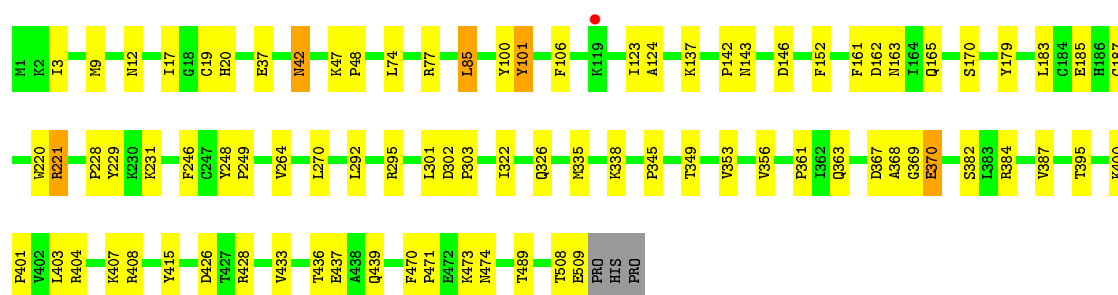
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Respiratory nitrate reductase 1 alpha chain

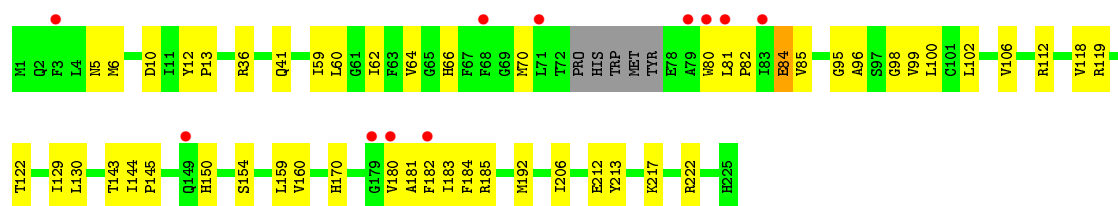
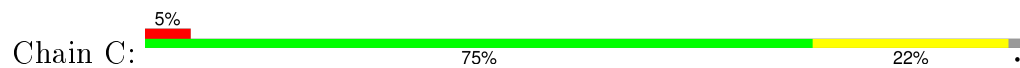


- Molecule 2: Respiratory nitrate reductase 1 beta chain





- Molecule 3: Respiratory nitrate reductase 1 gamma chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.45Å 240.69Å 139.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.30 49.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.61-2.30) 99.7 (49.84-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.200 , 0.237 0.195 , 0.230	Depositor DCC
$R_{free}$ test set	6894 reflections (6.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 114166 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: 6MO, FME, SF4, AGA, F3S, HEM, MD1

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	0.38	0/10123	0.66	6/13742 (0.0%)
2	B	0.36	0/4146	0.62	0/5609
3	C	0.42	0/1784	0.57	0/2411
All	All	0.38	0/16053	0.64	6/21762 (0.0%)

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	2	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	C-N-CA	12.74	153.56	121.70
1	A	501	ALA	C-N-CA	9.37	145.14	121.70
1	A	1163	HIS	CA-C-N	-6.47	102.95	117.20
1	A	501	ALA	N-CA-CB	6.20	118.78	110.10
1	A	809	LEU	N-CA-C	-5.50	96.15	111.00
1	A	720	SER	N-CA-C	5.13	124.84	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	ALA	CA
1	A	502	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9865	0	9522	205	0
2	B	4050	0	3973	56	0
3	C	1747	0	1789	33	0
4	A	94	0	42	11	0
5	A	1	0	0	0	0
6	A	8	0	0	1	0
6	B	24	0	0	2	0
7	A	25	0	29	0	0
8	B	7	0	0	0	0
9	C	86	0	60	3	0
10	A	253	0	0	5	2
10	B	182	0	0	4	0
10	C	34	0	0	0	0
All	All	16376	0	15415	287	2

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 9.

All (287) 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:338:MET:HE2	1:A:374:THR:HB	1.58	0.85
1:A:360:LEU:HG	1:A:383:MET:HE3	1.59	0.81
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.66	0.78
1:A:715:ASN:O	1:A:718:GLY:O	2.02	0.77
1:A:345:ARG:HB2	1:A:348:TYR:O	1.86	0.75
2:B:426:ASP:OD2	2:B:428:ARG:HD3	1.88	0.74
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.70	0.72
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:LYS:HD2	10:B:693:HOH:O	1.91	0.70
1:A:1098:HIS:CE1	4:A:1251:MD1:S13	2.85	0.69
1:A:401:ASN:HA	1:A:1034:PRO:HD3	1.77	0.67
1:A:402:LEU:HD13	1:A:1034:PRO:HB3	1.77	0.66
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.78	0.66
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.77	0.65
1:A:462:LEU:HD12	1:A:466:SER:OG	1.97	0.65
2:B:407:LYS:HG2	2:B:433:VAL:HG11	1.80	0.64
1:A:214:LEU:HB3	1:A:607:SER:OG	1.96	0.64
1:A:750:LYS:HD2	1:A:750:LYS:N	2.13	0.63
1:A:856:SER:O	1:A:859:GLU:HG2	1.98	0.63
1:A:578:VAL:HG23	1:A:579:GLY:H	1.64	0.63
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.15	0.62
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.80	0.62
1:A:282:PRO:HB2	1:A:1158:MET:HE3	1.80	0.61
1:A:1098:HIS:HE1	4:A:1251:MD1:S13	2.24	0.61
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.82	0.61
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.01	0.61
2:B:137:LYS:HA	10:B:667:HOH:O	2.00	0.61
1:A:191:ILE:HD12	1:A:191:ILE:H	1.65	0.60
2:B:370:GLU:HA	2:B:370:GLU:OE1	2.02	0.60
2:B:187:CYS:HB3	2:B:349:THR:O	2.02	0.60
1:A:223:LEU:O	1:A:225:PRO:HD3	2.00	0.60
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.22	0.60
2:B:407:LYS:HG2	2:B:433:VAL:CG1	2.31	0.59
1:A:49:CYS:HB3	1:A:791:TRP:CZ3	2.37	0.59
1:A:371:GLU:N	1:A:371:GLU:OE1	2.28	0.59
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.85	0.58
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.03	0.58
1:A:20:GLY:O	3:C:217:LYS:HD2	2.04	0.58
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.86	0.58
2:B:404:ARG:O	2:B:408:ARG:HG3	2.02	0.57
1:A:582:LYS:HD2	10:A:1497:HOH:O	2.04	0.57
1:A:190:PRO:HD3	1:A:714:SER:HB2	1.85	0.57
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.34	0.57
1:A:338:MET:CE	1:A:374:THR:HB	2.31	0.57
3:C:80:TRP:C	3:C:81:LEU:HG	2.24	0.57
1:A:719:SER:HB2	1:A:1099:SER:HB3	1.87	0.57
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.04	0.56
1:A:116:ARG:HE	1:A:147:SER:CB	2.19	0.56
3:C:6:MET:O	3:C:10:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HG2	1:A:516:SER:N	2.20	0.56
3:C:96:ALA:O	3:C:100:LEU:HD13	2.06	0.56
1:A:362:ASP:C	1:A:364:LEU:N	2.58	0.56
1:A:336:MET:HA	1:A:473:VAL:HB	1.88	0.55
1:A:750:LYS:CD	1:A:750:LYS:N	2.69	0.55
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.40	0.55
2:B:367:ASP:C	2:B:369:GLY:H	2.10	0.55
3:C:180:VAL:HG22	3:C:184:PHE:CD2	2.42	0.55
1:A:220:TYR:HD1	10:A:1469:HOH:O	1.90	0.55
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.89	0.55
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.88	0.55
1:A:1098:HIS:CE1	4:A:1247:MD1:S12	3.00	0.54
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.27	0.54
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.90	0.54
1:A:974:LEU:HD21	1:A:1033:ILE:HD13	1.88	0.54
1:A:417:LEU:O	1:A:472:THR:HG21	2.06	0.54
1:A:500:LYS:O	1:A:502:TYR:N	2.41	0.54
1:A:225:PRO:HB2	1:A:551:ASP:OD1	2.07	0.54
4:A:1247:MD1:H7	4:A:1247:MD1:C11	2.38	0.54
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.90	0.54
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.88	0.54
3:C:13:PRO:HG3	3:C:192:MET:SD	2.48	0.53
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.77	0.53
1:A:299:GLN:NE2	1:A:1158:MET:HB3	2.24	0.53
1:A:499:VAL:O	1:A:500:LYS:HG2	2.07	0.53
1:A:457:VAL:HG21	1:A:469:LEU:HD22	1.90	0.53
1:A:402:LEU:CD1	1:A:1034:PRO:HB3	2.38	0.53
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.43	0.53
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.44	0.53
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.24	0.53
1:A:191:ILE:O	1:A:194:MET:HG2	2.07	0.53
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.42	0.53
3:C:60:LEU:O	3:C:64:VAL:HG23	2.09	0.53
2:B:246:PHE:HA	6:B:803:SF4:S4	2.48	0.52
1:A:457:VAL:CG2	1:A:469:LEU:HD22	2.39	0.52
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.90	0.52
3:C:181:ALA:HB3	3:C:184:PHE:CE2	2.44	0.52
1:A:54:THR:HA	1:A:580:GLN:HG3	1.91	0.52
1:A:68:VAL:HB	1:A:102:LEU:HD22	1.91	0.52
1:A:578:VAL:HG23	1:A:579:GLY:N	2.25	0.51
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:HH11	1:A:331:ARG:HG3	1.76	0.51
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.45	0.51
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.91	0.51
1:A:804:PRO:O	1:A:1006:ILE:HG13	2.11	0.51
2:B:19:CYS:O	2:B:20:HIS:HB2	2.10	0.51
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:360:LEU:CG	1:A:383:MET:HE3	2.36	0.51
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.10	0.51
1:A:191:ILE:O	1:A:191:ILE:HG22	2.10	0.51
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.11	0.51
1:A:100:TRP:O	1:A:104:SER:HB3	2.10	0.51
1:A:864:LEU:N	1:A:864:LEU:HD22	2.25	0.50
1:A:914:LYS:O	1:A:914:LYS:HG2	2.11	0.50
1:A:338:MET:HE3	1:A:375:VAL:C	2.31	0.50
1:A:1243:GLU:O	1:A:1244:SER:O	2.29	0.50
1:A:371:GLU:H	1:A:371:GLU:CD	2.12	0.50
3:C:119:ARG:O	3:C:122:THR:HG22	2.11	0.50
4:A:1247:MD1:O11	4:A:1247:MD1:H7	2.12	0.50
1:A:400:TRP:CE2	1:A:1034:PRO:HG2	2.47	0.50
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.12	0.50
1:A:515:ARG:HG2	1:A:516:SER:H	1.77	0.50
1:A:49:CYS:HA	1:A:791:TRP:CE3	2.46	0.49
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.47	0.49
1:A:582:LYS:NZ	1:A:584:ARG:NH1	2.60	0.49
3:C:12:TYR:HB3	3:C:13:PRO:HD3	1.94	0.49
1:A:931:ASN:O	1:A:932:TYR:HB2	2.11	0.49
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	1.93	0.49
2:B:100:TYR:O	2:B:101:TYR:HB3	2.11	0.49
1:A:116:ARG:HE	1:A:147:SER:HB2	1.76	0.49
1:A:652:MET:CE	1:A:862:GLN:HE22	2.26	0.49
1:A:168:LEU:O	1:A:168:LEU:HD23	2.13	0.49
1:A:328:ASP:CG	1:A:332:ARG:HE	2.16	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.28	0.49
1:A:487:LEU:CD1	1:A:487:LEU:N	2.76	0.49
1:A:411:GLU:HG3	1:A:412:GLU:N	2.27	0.49
1:A:624:THR:O	1:A:627:GLU:HG2	2.12	0.48
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.95	0.48
3:C:102:LEU:O	3:C:106:VAL:HG23	2.14	0.48
1:A:220:TYR:CE1	4:A:1247:MD1:H101	2.49	0.48
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.96	0.48
1:A:490:VAL:O	1:A:500:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:GLN:HG2	2:B:382:SER:O	2.14	0.48
3:C:70:MET:HG2	3:C:160:VAL:HG22	1.96	0.48
1:A:1100:THR:OG1	4:A:1247:MD1:H5'1	2.14	0.47
3:C:59:ILE:HD13	9:C:806:HEM:HAC	1.95	0.47
2:B:220:TRP:C	2:B:221:ARG:HG3	2.34	0.47
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.96	0.47
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.15	0.47
1:A:1132:ASN:ND2	2:B:137:LYS:HE2	2.28	0.47
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.15	0.47
1:A:378:ASN:OD1	1:A:382:GLU:HB2	2.15	0.47
3:C:84:GLU:HG3	3:C:85:VAL:N	2.29	0.47
1:A:1098:HIS:CE1	4:A:1251:MD1:H15	2.33	0.47
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.29	0.47
1:A:173:ASN:O	1:A:177:ILE:HG13	2.14	0.47
3:C:150:HIS:HB3	3:C:154:SER:HG	1.80	0.47
1:A:578:VAL:CG2	1:A:579:GLY:H	2.26	0.47
1:A:1062:ARG:HD2	10:A:1476:HOH:O	2.14	0.47
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.50	0.47
2:B:3:ILE:HG12	2:B:301:LEU:CD1	2.45	0.47
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.45	0.46
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.50	0.46
1:A:1183:ILE:HG13	1:A:1185:ASN:H	1.79	0.46
1:A:33:ASP:O	1:A:37:GLN:HG3	2.16	0.46
2:B:335:MET:O	2:B:338:LYS:HE3	2.15	0.46
2:B:367:ASP:C	2:B:369:GLY:N	2.69	0.46
3:C:150:HIS:HB3	3:C:154:SER:OG	2.15	0.46
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.51	0.46
2:B:162:ASP:O	2:B:163:ASN:HB2	2.16	0.46
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.46	0.46
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.50	0.46
1:A:611:PHE:CD2	1:A:727:MET:HE1	2.51	0.46
1:A:279:ALA:HB2	1:A:291:CYS:SG	2.56	0.45
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.50	0.45
1:A:536:SER:HB2	1:A:566:CYS:SG	2.57	0.45
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.52	0.45
1:A:644:ASP:OD2	1:A:751:PRO:HB2	2.17	0.45
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.82	0.45
1:A:791:TRP:HZ3	1:A:1101:TYR:HH	1.62	0.45
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.32	0.45
3:C:182:PHE:O	3:C:185:ARG:N	2.50	0.45
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ARG:HA	2:B:295:ARG:HD2	1.81	0.45
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.52	0.45
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.52	0.44
3:C:143:THR:HB	3:C:184:PHE:CE1	2.51	0.44
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.52	0.44
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.17	0.44
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.99	0.44
1:A:487:LEU:N	1:A:487:LEU:HD12	2.33	0.44
1:A:641:HIS:O	1:A:644:ASP:HB2	2.17	0.44
1:A:384:VAL:HG22	1:A:385:ALA:N	2.33	0.44
2:B:9:MET:HE2	2:B:270:LEU:HD21	2.00	0.44
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.44
1:A:1068:ARG:HG3	1:A:1068:ARG:HH21	1.82	0.44
1:A:362:ASP:C	1:A:364:LEU:H	2.20	0.44
1:A:425:GLU:O	1:A:457:VAL:HG22	2.18	0.44
1:A:336:MET:N	1:A:337:PRO:HD2	2.33	0.44
1:A:729:LYS:HD3	1:A:730:TYR:CE1	2.53	0.44
1:A:6:ARG:O	1:A:9:TYR:N	2.49	0.44
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.82	0.43
2:B:302:ASP:HA	2:B:303:PRO:HD2	1.88	0.43
1:A:894:ALA:O	1:A:898:ARG:HG3	2.16	0.43
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.43
1:A:1152:GLN:OE1	2:B:170:SER:HA	2.19	0.43
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.18	0.43
1:A:584:ARG:HD3	1:A:1006:ILE:HG12	1.99	0.43
1:A:876:LEU:HD23	1:A:876:LEU:C	2.39	0.43
1:A:56:SER:HB2	1:A:800:SER:HB2	1.99	0.43
1:A:338:MET:CE	1:A:374:THR:CB	2.97	0.43
1:A:582:LYS:HZ2	1:A:584:ARG:HG2	1.83	0.43
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.54	0.43
3:C:95:GLY:O	3:C:99:VAL:HG23	2.19	0.43
1:A:1028:ASN:HA	1:A:1033:ILE:O	2.18	0.43
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.83	0.43
2:B:42:ASN:HB2	6:B:803:SF4:S1	2.59	0.42
1:A:652:MET:HE3	1:A:862:GLN:HE22	1.83	0.42
1:A:286:GLU:HG2	2:B:179:TYR:OH	2.19	0.42
1:A:591:PRO:HA	1:A:596:LEU:HB2	2.00	0.42
1:A:308:ALA:HB2	1:A:507:ALA:HB2	2.00	0.42
1:A:155:GLY:HA2	10:B:619:HOH:O	2.18	0.42
1:A:26:ASN:HB3	10:A:1496:HOH:O	2.18	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HA	1:A:271:ARG:HD3	2.00	0.42
2:B:12:ASN:HA	2:B:356:VAL:HB	2.01	0.42
1:A:772:ASP:C	1:A:788:THR:HG22	2.40	0.42
1:A:55:GLY:HA3	6:A:1249:SF4:S3	2.59	0.42
2:B:387:VAL:HG21	2:B:403:LEU:HG	2.01	0.42
2:B:508:THR:O	2:B:509:GLU:CB	2.67	0.42
3:C:41:GLN:HB2	9:C:806:HEM:O1A	2.20	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.19	0.42
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.19	0.42
3:C:129:ILE:CG2	3:C:130:LEU:N	2.82	0.42
1:A:1006:ILE:CD1	1:A:1016:GLU:CD	2.88	0.42
1:A:525:PHE:CZ	1:A:536:SER:HB3	2.55	0.42
1:A:340:VAL:O	1:A:470:VAL:HA	2.19	0.42
1:A:1023:ASN:O	1:A:1026:TYR:HB2	2.20	0.42
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.85	0.42
1:A:803:HIS:HB2	1:A:804:PRO:HD2	2.01	0.42
1:A:1037:THR:HA	1:A:1203:HIS:HB3	2.02	0.42
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.83	0.41
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.55	0.41
1:A:199:TYR:C	1:A:199:TYR:CD1	2.92	0.41
1:A:27:THR:HG23	3:C:222:ARG:HD3	2.01	0.41
1:A:116:ARG:HG3	1:A:120:MET:HE2	2.02	0.41
2:B:292:LEU:HD13	2:B:345:PRO:O	2.20	0.41
1:A:724:HIS:O	1:A:728:LEU:HD13	2.20	0.41
1:A:194:MET:HA	1:A:798:ASN:ND2	2.35	0.41
1:A:1006:ILE:HD13	1:A:1016:GLU:HG3	2.01	0.41
1:A:51:VAL:HB	1:A:791:TRP:CZ2	2.55	0.41
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.45	0.41
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.03	0.41
1:A:1091:PRO:O	1:A:1162:TYR:HA	2.20	0.41
1:A:54:THR:HA	1:A:580:GLN:CG	2.51	0.41
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.41
1:A:934:LYS:HD3	1:A:944:MET:SD	2.60	0.41
1:A:1068:ARG:HG3	1:A:1068:ARG:NH2	2.35	0.41
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.21	0.41
1:A:574:TRP:CZ2	1:A:576:HIS:HB2	2.55	0.41
1:A:489:ASP:HB3	1:A:492:CYS:SG	2.60	0.41
2:B:407:LYS:HG3	10:B:639:HOH:O	2.21	0.41
1:A:634:ASP:HB3	1:A:637:ARG:HG3	2.02	0.41
1:A:545:ASN:OD1	1:A:550:LEU:HD12	2.20	0.41
1:A:497:ASP:HA	1:A:505:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ARG:HH11	2:B:77:ARG:HB2	1.86	0.41
2:B:123:ILE:HG13	2:B:124:ALA:H	1.85	0.41
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.55	0.41
4:A:1247:MD1:O11	4:A:1247:MD1:C7	2.69	0.41
1:A:336:MET:HB3	1:A:474:TYR:HB2	2.02	0.41
1:A:218:ASP:N	1:A:218:ASP:OD2	2.54	0.41
1:A:289:LYS:O	1:A:289:LYS:HD3	2.21	0.41
1:A:1100:THR:HG1	4:A:1247:MD1:H5'1	1.85	0.41
1:A:261:THR:HG23	2:B:17:ILE:HD12	2.02	0.41
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.55	0.41
1:A:231:TRP:CD1	1:A:1042:GLN:HG2	2.56	0.41
3:C:159:LEU:H	3:C:159:LEU:HD22	1.86	0.41
2:B:101:TYR:CZ	2:B:142:PRO:HD3	2.56	0.40
1:A:378:ASN:OD1	1:A:382:GLU:N	2.54	0.40
2:B:508:THR:O	2:B:509:GLU:HB3	2.20	0.40
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.36	0.40
2:B:231:LYS:HD3	2:B:231:LYS:HA	1.73	0.40
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.51	0.40
2:B:436:THR:OG1	2:B:439:GLN:HG3	2.21	0.40
3:C:12:TYR:N	3:C:13:PRO:CD	2.84	0.40
1:A:1048:HIS:O	1:A:1049:GLN:C	2.59	0.40
2:B:322:ILE:O	2:B:326:GLN:HG3	2.22	0.40
1:A:191:ILE:HA	1:A:192:PRO:HD2	1.97	0.40
1:A:37:GLN:HB3	10:A:1450:HOH:O	2.22	0.40
2:B:47:LYS:HA	2:B:48:PRO:C	2.41	0.40
1:A:806:ILE:HG23	1:A:806:ILE:O	2.21	0.40
3:C:112:ARG:HA	3:C:118:VAL:CG1	2.51	0.40
1:A:717:LEU:HG	1:A:778:THR:HG23	2.03	0.40
1:A:363:ALA:O	1:A:366:GLN:HB2	2.22	0.40
1:A:713:ARG:HA	4:A:1247:MD1:C4	2.51	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CE2	2.56	0.40
1:A:696:ALA:O	1:A:699:PRO:HD3	2.22	0.40
3:C:62:ILE:HD11	3:C:98:GLY:HA2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1489:HOH:O	10:A:1489:HOH:O[3_354]	1.16	1.04
10:A:1450:HOH:O	10:A:1450:HOH:O[3_354]	1.59	0.61

## 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	1242/1247 (100%)	1162 (94%)	71 (6%)	9 (1%)	26	31
2	B	507/512 (99%)	492 (97%)	13 (3%)	2 (0%)	39	48
3	C	216/225 (96%)	202 (94%)	14 (6%)	0	100	100
All	All	1965/1984 (99%)	1856 (94%)	98 (5%)	11 (1%)	30	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	502	TYR
1	A	1166	GLU
1	A	578	VAL
1	A	1164	ALA
1	A	720	SER
2	B	101	TYR
1	A	191	ILE
1	A	224	PRO
2	B	368	ALA
1	A	195	SER

### 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	1039/1044 (100%)	1009 (97%)	30 (3%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	436/439 (99%)	427 (98%)	9 (2%)	61	78
3	C	180/186 (97%)	175 (97%)	5 (3%)	51	68
All	All	1655/1669 (99%)	1611 (97%)	44 (3%)	52	70

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	94	ARG
1	A	371	GLU
1	A	383	MET
1	A	402	LEU
1	A	461	GLN
1	A	467	THR
1	A	476	LEU
1	A	483	LEU
1	A	502	TYR
1	A	515	ARG
1	A	533	HIS
1	A	586	GLN
1	A	626	GLU
1	A	663	THR
1	A	673	GLU
1	A	717	LEU
1	A	727	MET
1	A	743	LEU
1	A	750	LYS
1	A	767	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	1006	ILE
1	A	1041	ARG
1	A	1087	ASN
1	A	1110	LEU
1	A	1233	LEU
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU

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Mol	Chain	Res	Type
2	B	161	PHE
2	B	165	GLN
2	B	183	LEU
2	B	221	ARG
2	B	370	GLU
3	C	36	ARG
3	C	66	HIS
3	C	84	GLU
3	C	170	HIS
3	C	212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	173	ASN
1	A	234	GLN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	599	GLN
1	A	708	ASN
1	A	946	ASN
1	A	1098	HIS
2	B	143	ASN
3	C	149	GLN
3	C	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	FME	C	1	3	8,9,10	1.59	2 (25%)	6,9,11	1.93	2 (33%)

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	FME	C	1	3	-	0/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-3.38	1.47	1.53
3	C	1	FME	CA-N	-2.04	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	O1-CN-N	-3.17	120.19	124.76
3	C	1	FME	CA-N-CN	2.51	126.68	122.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MD1	A	1247	5	39,51,51	3.90	10 (25%)	37,78,78	2.39	10 (27%)
6	SF4	A	1249	1	0,12,12	0.00	-	0,24,24	0.00	-
7	AGA	A	1250	-	24,24,29	0.76	1 (4%)	28,29,35	1.44	2 (7%)
4	MD1	A	1251	5	39,51,51	3.64	11 (28%)	37,78,78	2.31	11 (29%)
6	SF4	B	802	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	B	803	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	B	804	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	805	2	0,9,9	0.00	-	0,15,15	0.00	-
9	HEM	C	806	3	30,50,50	2.31	10 (33%)	24,82,82	2.67	10 (41%)
9	HEM	C	807	3	30,50,50	2.42	12 (40%)	24,82,82	2.78	11 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MD1	A	1247	5	-	0/18/59/59	0/5/5/5
6	SF4	A	1249	1	-	0/0/48/48	0/6/5/5
7	AGA	A	1250	-	-	0/26/26/34	0/0/0/0
4	MD1	A	1251	5	-	0/18/59/59	0/5/5/5
6	SF4	B	802	2	-	0/0/48/48	0/6/5/5
6	SF4	B	803	2	-	0/0/48/48	0/6/5/5
6	SF4	B	804	2	-	0/0/48/48	0/6/5/5
8	F3S	B	805	2	-	0/0/24/24	0/0/3/3
9	HEM	C	806	3	-	0/10/54/54	0/0/8/8
9	HEM	C	807	3	-	0/10/54/54	0/0/8/8

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	806	HEM	C2D-C3D	-6.37	1.35	1.54
9	C	807	HEM	C2D-C3D	-5.94	1.36	1.54
9	C	806	HEM	C3B-C4B	-4.82	1.47	1.51
9	C	807	HEM	C3B-C4B	-4.37	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	806	HEM	C3D-C4D	-3.10	1.47	1.51
9	C	806	HEM	C2C-C1C	-2.96	1.47	1.52
9	C	807	HEM	C3D-C4D	-2.75	1.48	1.51
9	C	807	HEM	C2C-C1C	-2.68	1.47	1.52
9	C	807	HEM	CAD-C3D	2.18	1.58	1.54
9	C	806	HEM	C1C-NC	2.23	1.38	1.36
4	A	1251	MD1	C4-N3	2.29	1.39	1.35
4	A	1251	MD1	O11-C11	2.35	1.48	1.42
7	A	1250	AGA	C8-C7	2.42	1.57	1.50
9	C	807	HEM	CMA-C3A	2.46	1.56	1.51
9	C	806	HEM	FE-NC	2.46	2.05	1.95
4	A	1247	MD1	C14-C13	2.47	1.53	1.50
9	C	806	HEM	CMA-C3A	2.50	1.56	1.51
4	A	1251	MD1	O4'-C1'	2.51	1.44	1.41
4	A	1251	MD1	C2-N1	2.52	1.39	1.35
4	A	1247	MD1	C13-C12	2.61	1.42	1.34
9	C	807	HEM	FE-NC	2.77	2.06	1.95
4	A	1251	MD1	C20-N18	2.82	1.39	1.35
9	C	807	HEM	C3C-CAC	2.86	1.56	1.51
9	C	806	HEM	C4C-NC	2.86	1.39	1.36
9	C	806	HEM	C3C-CAC	2.88	1.56	1.51
4	A	1247	MD1	C20-N18	2.88	1.39	1.35
4	A	1251	MD1	C17-N17	2.92	1.40	1.35
4	A	1251	MD1	C16-C20	2.96	1.45	1.40
9	C	807	HEM	C1C-NC	3.01	1.39	1.36
4	A	1247	MD1	C2-N1	3.13	1.40	1.35
9	C	807	HEM	CAA-C2A	3.24	1.57	1.52
4	A	1247	MD1	C4-N3	3.29	1.40	1.35
4	A	1247	MD1	C17-N17	3.52	1.41	1.35
4	A	1251	MD1	C14-N15	3.85	1.51	1.47
9	C	806	HEM	C3B-CAB	4.02	1.58	1.51
9	C	807	HEM	C3B-CAB	4.33	1.59	1.51
9	C	807	HEM	C4C-NC	4.34	1.41	1.36
4	A	1247	MD1	C6-N1	4.63	1.41	1.33
4	A	1251	MD1	C15-N17	5.04	1.42	1.33
4	A	1247	MD1	C15-N17	5.11	1.42	1.33
4	A	1251	MD1	C6-N1	5.14	1.42	1.33
4	A	1247	MD1	C16-C20	5.76	1.48	1.40
4	A	1251	MD1	C7-N8	19.25	1.49	1.27
4	A	1247	MD1	C7-N8	20.81	1.50	1.27

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C5-C6-N1	-6.43	114.79	123.59
4	A	1251	MD1	C5-C6-N1	-5.39	116.22	123.59
4	A	1251	MD1	N3-C2-N1	-5.25	119.45	127.44
9	C	807	HEM	C3C-CAC-CBC	-4.35	117.79	124.46
4	A	1247	MD1	N17-C17-N18	-4.32	118.46	125.53
4	A	1247	MD1	N3-C2-N1	-4.12	121.17	127.44
9	C	806	HEM	C3C-CAC-CBC	-3.76	118.69	124.46
4	A	1251	MD1	O3B-PB-O3A	-3.76	92.97	102.94
4	A	1251	MD1	N17-C17-N18	-3.57	119.69	125.53
9	C	807	HEM	CAA-C2A-C1A	-3.09	123.65	127.01
9	C	807	HEM	CMA-C3A-C4A	-3.09	123.26	128.36
4	A	1251	MD1	C6-C5-C4	-3.08	117.22	120.90
4	A	1247	MD1	C6-C5-C4	-2.97	117.34	120.90
4	A	1247	MD1	O3B-PA-O5'	-2.84	95.41	102.94
9	C	806	HEM	CMA-C3A-C4A	-2.80	123.73	128.36
9	C	806	HEM	CAA-C2A-C1A	-2.59	124.19	127.01
4	A	1247	MD1	C1'-N9-C4	-2.53	123.13	126.94
4	A	1251	MD1	C1'-N9-C4	-2.07	123.82	126.94
9	C	807	HEM	CAD-C3D-C4D	2.11	119.90	112.47
9	C	806	HEM	CMA-C3A-C2A	2.21	129.87	125.24
4	A	1251	MD1	N16-C17-N17	2.22	120.87	117.20
9	C	807	HEM	CAA-CBA-CGA	2.25	116.86	112.75
4	A	1251	MD1	O4'-C1'-N9	2.25	112.82	108.10
4	A	1247	MD1	N2-C2-N3	2.27	122.16	117.80
9	C	806	HEM	CAD-C3D-C4D	2.32	120.66	112.47
9	C	807	HEM	CMA-C3A-C2A	2.45	130.36	125.24
4	A	1247	MD1	N16-C17-N18	2.94	122.07	117.20
9	C	807	HEM	CMD-C2D-C3D	3.16	128.32	114.35
9	C	806	HEM	CMD-C2D-C3D	3.27	128.82	114.35
4	A	1251	MD1	PA-O3B-PB	3.42	142.33	132.73
9	C	806	HEM	C2D-C3D-C4D	3.73	107.82	101.50
9	C	807	HEM	C2D-C3D-C4D	3.86	108.05	101.50
7	A	1250	AGA	C9-C8-C7	4.60	131.69	113.59
7	A	1250	AGA	C14-C13-C12	4.63	131.78	113.59
9	C	806	HEM	CMC-C2C-C3C	4.80	128.51	116.53
9	C	807	HEM	CMC-C2C-C3C	4.85	128.64	116.53
4	A	1251	MD1	C15-N17-C17	5.04	122.94	115.94
9	C	807	HEM	CMB-C2B-C3B	5.43	130.09	116.53
4	A	1251	MD1	C6-N1-C2	5.44	123.49	115.94
9	C	806	HEM	CMB-C2B-C3B	5.48	130.21	116.53
4	A	1247	MD1	C15-N17-C17	5.91	124.15	115.94
9	C	806	HEM	CAD-C3D-C2D	6.37	131.52	113.22
9	C	807	HEM	CAD-C3D-C2D	6.55	132.05	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C6-N1-C2	6.56	125.05	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1247	MD1	8	0
6	A	1249	SF4	1	0
4	A	1251	MD1	3	0
6	B	803	SF4	2	0
9	C	806	HEM	3	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	1244/1247 (99%)	-0.05	44 (3%) 48 56	19, 34, 49, 58	0
2	B	509/512 (99%)	-0.48	1 (0%) 95 97	19, 28, 41, 57	0
3	C	219/225 (97%)	-0.06	11 (5%) 32 41	22, 39, 53, 58	0
All	All	1972/1984 (99%)	-0.16	56 (2%) 56 66	19, 33, 49, 58	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	80	TRP	6.0
1	A	9	TYR	5.5
1	A	10	PHE	5.5
3	C	79	ALA	4.5
1	A	221	CYS	3.9
1	A	223	LEU	3.7
1	A	462	LEU	3.6
1	A	348	TYR	3.6
1	A	460	LEU	3.5
1	A	361	VAL	3.4
2	B	119	LYS	3.3
3	C	182	PHE	3.1
1	A	461	GLN	3.1
1	A	7	PHE	3.1
1	A	717	LEU	3.0
3	C	180	VAL	3.0
1	A	1215	GLY	2.9
3	C	71	LEU	2.9
3	C	81	LEU	2.8
3	C	83	ILE	2.7
3	C	3	PHE	2.7
1	A	465	GLY	2.7
1	A	578	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	179	GLY	2.7
1	A	875	ASP	2.7
1	A	11	LYS	2.6
3	C	68	PHE	2.6
1	A	225	PRO	2.6
1	A	346	ASP	2.6
1	A	220	TYR	2.6
1	A	719	SER	2.5
1	A	347	GLY	2.5
1	A	759	ASN	2.4
1	A	1214	VAL	2.4
1	A	679	PRO	2.4
1	A	349	TYR	2.4
1	A	467	THR	2.4
1	A	1216	SER	2.3
1	A	685	LYS	2.3
1	A	55	GLY	2.3
1	A	469	LEU	2.3
1	A	458	LYS	2.3
1	A	216	PHE	2.2
1	A	544	LEU	2.2
1	A	217	TYR	2.2
1	A	459	ARG	2.1
1	A	345	ARG	2.1
3	C	149	GLN	2.1
1	A	488	ASN	2.1
1	A	575	ALA	2.1
1	A	675	ALA	2.1
1	A	674	LYS	2.1
1	A	718	GLY	2.0
1	A	8	ARG	2.0
1	A	676	GLY	2.0
1	A	543	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	FME	C	1	10/11	0.93	0.28	-	53,57,63,64	0

### 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
7	AGA	A	1250	25/30	0.94	0.15	1.62	34,38,47,48	0
9	HEM	C	806	43/43	0.97	0.11	0.67	25,28,30,35	0
9	HEM	C	807	43/43	0.94	0.13	0.47	44,46,53,56	0
8	F3S	B	805	7/7	0.99	0.12	0.27	26,26,28,28	0
6	SF4	B	803	8/8	0.99	0.13	0.09	19,22,24,24	0
4	MD1	A	1251	47/47	0.95	0.17	-0.27	26,39,53,56	0
4	MD1	A	1247	47/47	0.93	0.15	-0.39	30,38,58,65	0
5	6MO	A	1248	1/1	0.93	0.16	-0.97	61,61,61,61	0
6	SF4	B	802	8/8	0.97	0.10	-1.26	26,28,30,32	0
6	SF4	B	804	8/8	0.94	0.08	-1.46	31,35,37,37	0
6	SF4	A	1249	8/8	0.96	0.07	-2.27	31,31,33,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.