



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:05 AM GMT

PDB ID : 3O0R  
Title : Crystal structure of nitric oxide reductase from *Pseudomonas aeruginosa* in complex with antibody fragment  
Authors : Hino, T.; Matsumoto, Y.; Nagano, S.; Sugimoto, H.; Fukumori, Y.; Murata, T.; Iwata, S.; Shiro, Y.  
Deposited on : 2010-07-20  
Resolution : 2.70 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

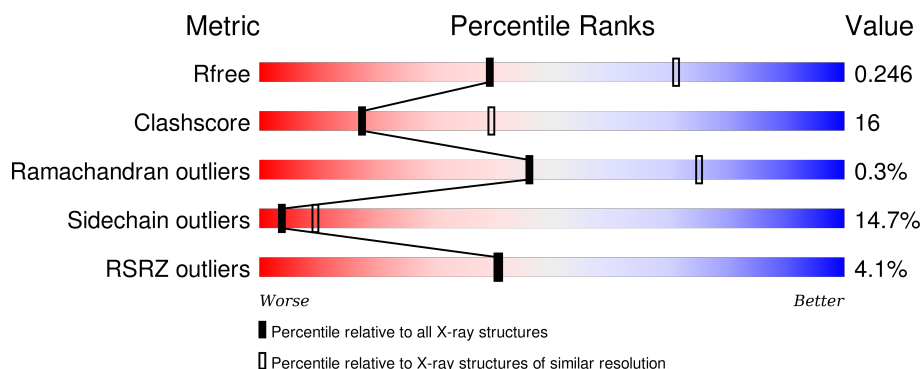
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	L	213	 6% 72% 23% 5%
2	H	225	 5% 70% 24% 5%
3	B	465	 3% 59% 30% 8% •
4	C	146	 3% 64% 29% • •

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8364 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 antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	SEE REMARK 999	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

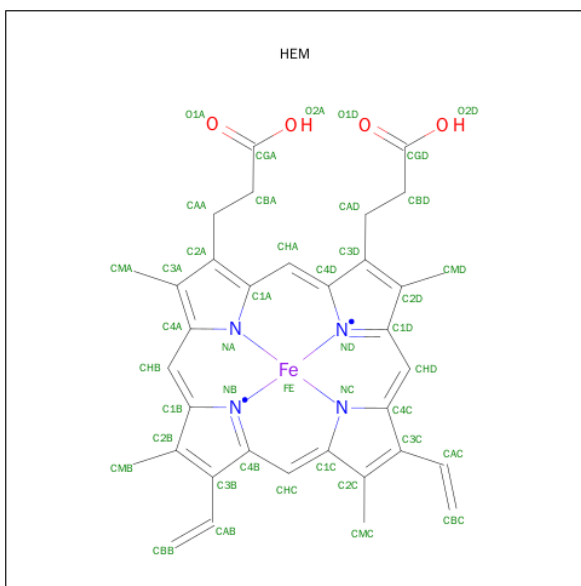
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	CONFLICT	UNP Q59646

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Fe 1 1	0	0

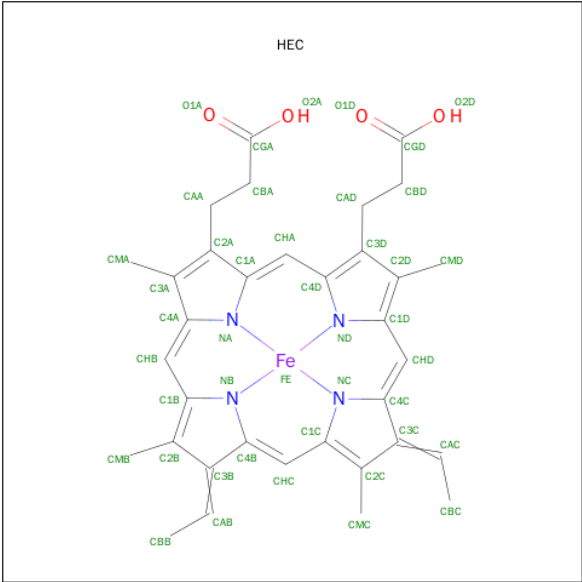
- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O 1 1	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



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

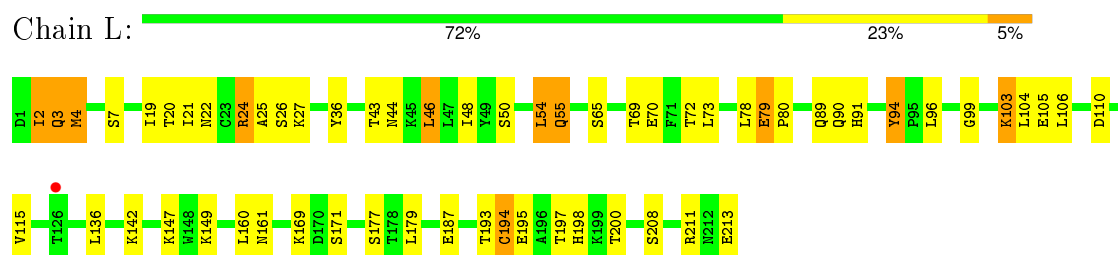
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	44	Total	O	0	0
			44	44		
10	H	46	Total	O	0	0
			46	46		
10	B	38	Total	O	0	0
			38	38		
10	C	44	Total	O	0	0
			44	44		

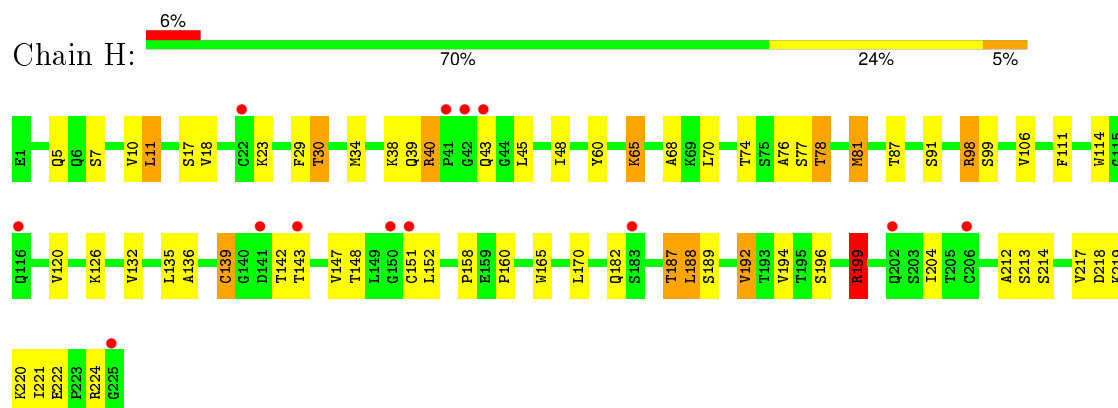
### 3 Residue-property plots [i](#)

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.

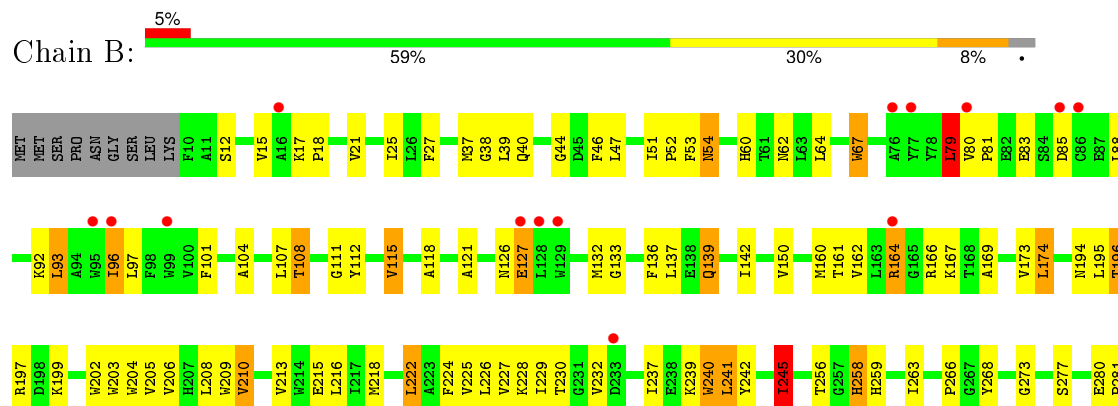
- Molecule 1: antibody fab fragment light chain

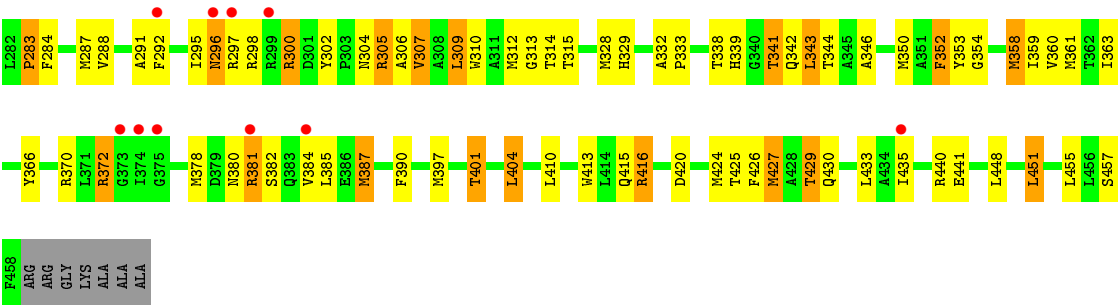


- Molecule 2: antibody fab fragment heavy chain

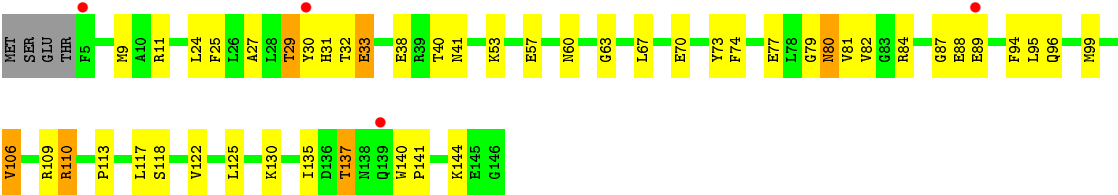


- Molecule 3: Nitric oxide reductase subunit B





● Molecule 4: Nitric oxide reductase subunit C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.47Å 104.52Å 195.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.70) 97.5 (20.00-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.247 0.185 , 0.246	Depositor DCC
$R_{free}$ test set	2559 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.8	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	0 of 50228 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: HEM, CA, FE, O, HEC

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	L	0.95	2/1709 (0.1%)	0.94	1/2317 (0.0%)
2	H	0.92	1/1735 (0.1%)	0.95	4/2367 (0.2%)
3	B	0.81	0/3693	0.86	6/5039 (0.1%)
4	C	0.94	2/1153 (0.2%)	0.89	1/1559 (0.1%)
All	All	0.88	5/8290 (0.1%)	0.90	12/11282 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	73	TYR	CE1-CZ	6.88	1.47	1.38
1	L	194	CYS	CB-SG	-6.17	1.71	1.82
4	C	94	PHE	CD2-CE2	5.57	1.50	1.39
2	H	151	CYS	CB-SG	-5.54	1.72	1.81
1	L	105	GLU	CG-CD	5.06	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	416	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	B	416	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	L	110	ASP	CB-CG-OD1	6.56	124.20	118.30
3	B	79	LEU	CA-CB-CG	6.45	130.14	115.30
2	H	218	ASP	CB-CG-OD1	6.06	123.76	118.30
3	B	420	ASP	CB-CG-OD2	-5.79	113.09	118.30
3	B	245	ILE	CB-CA-C	-5.70	100.20	111.60
4	C	110	ARG	NE-CZ-NH2	-5.70	117.45	120.30
3	B	174	LEU	CA-CB-CG	5.65	128.30	115.30
2	H	192	VAL	CB-CA-C	-5.36	101.21	111.40
2	H	199	ARG	CG-CD-NE	-5.33	100.60	111.80
2	H	81	MET	CG-SD-CE	-5.28	91.75	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1669	0	1606	45	0
2	H	1692	0	1647	37	0
3	B	3576	0	3619	147	0
4	C	1123	0	1092	46	0
5	B	86	0	60	8	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	C	1	0	0	0	0
9	C	43	0	30	6	0
10	B	38	0	0	3	0
10	C	44	0	0	2	0
10	H	46	0	0	6	0
10	L	44	0	0	3	0
All	All	8364	0	8054	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (260) 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)
2:H:182:GLN:HE21	2:H:187:THR:HG21	1.03	1.12
3:B:372:ARG:HG2	3:B:372:ARG:HH11	1.14	1.09
3:B:226:LEU:O	3:B:230:THR:HG22	1.56	1.05
3:B:104:ALA:O	3:B:108:THR:HG22	1.61	1.01
3:B:121:ALA:HA	3:B:132:MET:HE1	1.02	1.00
3:B:127:GLU:OE2	3:B:127:GLU:HA	1.62	0.99
3:B:121:ALA:CA	3:B:132:MET:HE1	1.93	0.98
2:H:30:THR:HB	10:H:338:HOH:O	1.64	0.97
3:B:300:ARG:HG3	3:B:300:ARG:HH11	1.31	0.91
3:B:425:THR:O	3:B:429:THR:HG23	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:182:GLN:NE2	2:H:187:THR:HG21	1.87	0.88
3:B:384:VAL:HA	3:B:387:MET:HE2	1.54	0.88
3:B:121:ALA:HA	3:B:132:MET:CE	1.98	0.86
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.57	0.85
4:C:106:VAL:HG22	4:C:109:ARG:HB2	1.60	0.83
3:B:338:THR:O	3:B:341:THR:HB	1.79	0.82
2:H:165:TRP:HZ3	2:H:221:ILE:HD11	1.42	0.81
3:B:350:MET:HB2	3:B:401:THR:HG21	1.63	0.81
1:L:79:GLU:CG	1:L:80:PRO:HD2	2.11	0.80
3:B:314:THR:HG23	3:B:358:MET:HB2	1.63	0.79
9:C:201:HEC:CGA	10:C:332:HOH:O	2.31	0.78
3:B:126:ASN:HB2	3:B:132:MET:HE2	1.66	0.78
3:B:225:VAL:O	3:B:229:ILE:HB	1.84	0.77
1:L:79:GLU:HG2	1:L:80:PRO:HD2	1.66	0.77
2:H:182:GLN:HE21	2:H:187:THR:CG2	1.93	0.77
3:B:381:ARG:HH11	3:B:381:ARG:HB3	1.48	0.77
4:C:88:GLU:HG3	4:C:89:GLU:N	2.00	0.75
4:C:137:THR:HG21	4:C:140:TRP:O	1.87	0.75
1:L:79:GLU:HG3	1:L:80:PRO:CD	2.18	0.74
1:L:79:GLU:CG	1:L:80:PRO:CD	2.66	0.73
3:B:104:ALA:O	3:B:108:THR:CG2	2.36	0.73
3:B:162:VAL:O	3:B:167:LYS:HE3	1.88	0.72
2:H:38:LYS:HE2	2:H:40:ARG:HD3	1.71	0.72
4:C:84:ARG:O	4:C:84:ARG:HG2	1.88	0.72
3:B:341:THR:HG22	3:B:343:LEU:H	1.55	0.71
3:B:372:ARG:NH1	3:B:372:ARG:HG2	1.93	0.71
1:L:79:GLU:HG3	1:L:80:PRO:HD3	1.72	0.71
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.05	0.71
1:L:160:LEU:HD11	2:H:182:GLN:HG2	1.72	0.70
4:C:88:GLU:HG3	4:C:89:GLU:H	1.55	0.70
3:B:304:ASN:OD1	3:B:306:ALA:HB3	1.91	0.70
3:B:85:ASP:HB2	3:B:166:ARG:HG3	1.74	0.70
2:H:65:LYS:HA	2:H:65:LYS:HE2	1.73	0.70
4:C:113:PRO:HD3	9:C:201:HEC:CBC	2.22	0.69
3:B:93:LEU:O	3:B:97:LEU:HG	1.92	0.69
4:C:25:PHE:O	4:C:29:THR:HG23	1.93	0.68
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.26	0.68
3:B:196:THR:HG22	4:C:135:ILE:HD13	1.77	0.67
3:B:51:ILE:O	3:B:51:ILE:HG22	1.95	0.66
3:B:300:ARG:HG3	3:B:300:ARG:NH1	2.05	0.65
2:H:165:TRP:HZ3	2:H:221:ILE:CD1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:113:PRO:HD3	9:C:201:HEC:HBC2	1.76	0.65
2:H:76:ALA:O	2:H:78:THR:HG22	1.97	0.65
2:H:60:TYR:CD2	2:H:65:LYS:HE3	2.33	0.64
1:L:115:VAL:HG22	1:L:136:LEU:HD23	1.79	0.63
3:B:126:ASN:HB2	3:B:132:MET:CE	2.27	0.63
3:B:353:TYR:N	5:B:801:HEM:HBC1	2.14	0.63
3:B:199:LYS:HG2	4:C:70:GLU:OE1	1.98	0.63
3:B:381:ARG:NH1	3:B:381:ARG:HB3	2.14	0.62
3:B:83:GLU:HA	3:B:83:GLU:OE2	2.00	0.62
3:B:222:LEU:HD12	3:B:287:MET:CE	2.29	0.62
3:B:266:PRO:HD2	4:C:32:THR:HG23	1.80	0.62
2:H:220:LYS:HE3	2:H:222:GLU:OE2	2.00	0.61
3:B:67:TRP:HZ3	3:B:360:VAL:HG11	1.65	0.61
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.66	0.60
3:B:196:THR:CG2	4:C:135:ILE:HD13	2.31	0.60
3:B:230:THR:HG23	3:B:232:VAL:H	1.66	0.60
3:B:295:ILE:HG23	3:B:295:ILE:O	2.00	0.60
1:L:48:ILE:HD13	1:L:54:LEU:HD23	1.82	0.60
3:B:425:THR:O	3:B:429:THR:CG2	2.49	0.60
3:B:291:ALA:HB2	3:B:315:THR:HG21	1.84	0.60
3:B:126:ASN:CB	3:B:132:MET:HE2	2.32	0.60
3:B:230:THR:OG1	3:B:232:VAL:HG23	2.03	0.59
3:B:197:ARG:HD3	4:C:33:GLU:OE2	2.03	0.59
3:B:341:THR:CG2	3:B:343:LEU:H	2.16	0.59
4:C:82:VAL:HG21	4:C:130:LYS:HA	1.85	0.58
2:H:74:THR:HG23	10:H:336:HOH:O	2.03	0.58
3:B:372:ARG:CG	3:B:372:ARG:HH11	2.01	0.58
2:H:165:TRP:CZ3	2:H:221:ILE:HD11	2.33	0.58
4:C:137:THR:CG2	4:C:140:TRP:O	2.52	0.58
1:L:50:SER:H	1:L:91:HIS:HE1	1.50	0.57
3:B:397:MET:O	3:B:401:THR:HG23	2.04	0.57
3:B:205:VAL:O	3:B:209:TRP:HB2	2.04	0.57
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.85	0.57
1:L:46:LEU:HD13	1:L:55:GLN:CG	2.36	0.56
1:L:3:GLN:HG2	1:L:26:SER:HB3	1.87	0.56
3:B:341:THR:HG22	3:B:343:LEU:N	2.20	0.56
4:C:84:ARG:NH1	9:C:201:HEC:O2A	2.35	0.56
3:B:139:GLN:NE2	3:B:139:GLN:H	2.03	0.56
3:B:430:GLN:NE2	4:C:110:ARG:HH12	2.04	0.56
1:L:160:LEU:CD1	2:H:182:GLN:HG2	2.34	0.56
1:L:24:ARG:HG3	1:L:25:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:17:LYS:HB3	3:B:18:PRO:CD	2.36	0.56
2:H:30:THR:CB	10:H:338:HOH:O	2.37	0.56
3:B:136:PHE:O	3:B:137:LEU:HD23	2.06	0.55
1:L:19:ILE:O	1:L:19:ILE:HD12	2.05	0.55
1:L:2:ILE:HG23	10:L:305:HOH:O	2.05	0.55
3:B:415:GLN:HB2	3:B:429:THR:HG21	1.88	0.55
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.36	0.55
3:B:21:VAL:O	3:B:25:ILE:HG12	2.08	0.54
2:H:29:PHE:CD1	2:H:77:SER:HA	2.42	0.54
1:L:198:HIS:CD2	1:L:200:THR:OG1	2.49	0.54
1:L:161:ASN:ND2	1:L:177:SER:OG	2.41	0.53
3:B:222:LEU:HD12	3:B:287:MET:HE1	1.91	0.53
3:B:93:LEU:HA	3:B:96:ILE:HG22	1.91	0.53
3:B:314:THR:HG23	3:B:358:MET:CB	2.34	0.52
3:B:118:ALA:O	3:B:121:ALA:HB3	2.08	0.52
3:B:226:LEU:O	3:B:230:THR:CG2	2.45	0.52
1:L:4:MET:HB3	1:L:99:GLY:HA2	1.91	0.52
3:B:38:GLY:HA3	3:B:441:GLU:OE1	2.08	0.52
2:H:40:ARG:NH1	10:H:319:HOH:O	2.43	0.52
2:H:70:LEU:HD21	2:H:81:MET:CE	2.39	0.52
4:C:96:GLN:HA	4:C:96:GLN:NE2	2.25	0.52
3:B:197:ARG:CD	4:C:33:GLU:OE2	2.57	0.52
4:C:77:GLU:OE1	4:C:79:GLY:HA3	2.10	0.52
10:H:338:HOH:O	3:B:424:MET:HE3	2.10	0.51
3:B:258:HIS:HD1	3:B:277:SER:HG	1.58	0.51
1:L:193:THR:HA	1:L:208:SER:HB3	1.92	0.51
3:B:202:TRP:CH2	3:B:206:VAL:HG21	2.44	0.51
1:L:46:LEU:HB3	1:L:55:GLN:HG3	1.92	0.51
3:B:339:HIS:HA	5:B:802:HEM:O1D	2.10	0.50
2:H:11:LEU:HD21	2:H:158:PRO:HG3	1.93	0.50
3:B:283:PRO:O	3:B:287:MET:HG3	2.11	0.50
3:B:378:MET:HB3	3:B:382:SER:HB2	1.93	0.50
3:B:196:THR:HB	3:B:263:ILE:O	2.12	0.50
3:B:350:MET:O	3:B:354:GLY:N	2.41	0.50
1:L:4:MET:CA	1:L:4:MET:CE	2.89	0.50
1:L:21:ILE:HD11	1:L:73:LEU:HD23	1.93	0.50
3:B:203:TRP:CE2	3:B:259:HIS:HB3	2.47	0.50
3:B:142:ILE:HG12	10:B:926:HOH:O	2.11	0.50
3:B:111:GLY:O	3:B:115:VAL:HG13	2.11	0.50
3:B:424:MET:HG2	3:B:429:THR:HG22	1.94	0.50
1:L:50:SER:H	1:L:91:HIS:CE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:ASN:HB3	3:B:197:ARG:NH1	2.27	0.49
1:L:4:MET:CE	1:L:4:MET:N	2.76	0.49
3:B:242:TYR:CZ	4:C:11:ARG:HG3	2.47	0.49
1:L:70:GLU:HG3	10:L:327:HOH:O	2.13	0.49
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.94	0.49
3:B:342:GLN:OE1	10:B:935:HOH:O	2.20	0.49
3:B:204:TRP:HZ2	4:C:29:THR:HG21	1.78	0.49
3:B:273:GLY:O	3:B:277:SER:HB2	2.12	0.49
3:B:390:PHE:CD1	3:B:390:PHE:C	2.86	0.49
3:B:126:ASN:CG	3:B:132:MET:HE2	2.33	0.49
3:B:341:THR:HG22	3:B:343:LEU:HB2	1.94	0.49
2:H:48:ILE:HG21	2:H:81:MET:HE3	1.94	0.49
4:C:80:ASN:H	4:C:80:ASN:HD22	1.60	0.49
3:B:230:THR:HG23	3:B:232:VAL:N	2.28	0.48
3:B:173:VAL:HG11	3:B:241:LEU:HD11	1.94	0.48
3:B:127:GLU:OE2	3:B:127:GLU:CA	2.46	0.48
1:L:46:LEU:HD13	1:L:55:GLN:HG3	1.94	0.48
3:B:216:LEU:HD11	3:B:245:ILE:CG2	2.44	0.48
4:C:113:PRO:HD3	9:C:201:HEC:HBC3	1.94	0.48
3:B:382:SER:HB3	3:B:457:SER:O	2.14	0.48
3:B:79:LEU:HD22	3:B:80:VAL:N	2.28	0.48
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.62	0.48
1:L:4:MET:CA	1:L:4:MET:HE2	2.43	0.48
1:L:4:MET:HE3	1:L:4:MET:N	2.29	0.48
2:H:132:VAL:HG21	2:H:217:VAL:HG21	1.96	0.48
3:B:359:ILE:HG23	3:B:360:VAL:N	2.28	0.48
3:B:332:ALA:HB3	3:B:333:PRO:HD3	1.95	0.47
3:B:300:ARG:NH1	3:B:300:ARG:CG	2.74	0.47
3:B:204:TRP:O	3:B:208:LEU:HB2	2.14	0.47
3:B:37:MET:HE1	3:B:60:HIS:CG	2.50	0.47
3:B:218:MET:HG3	3:B:359:ILE:HD13	1.95	0.47
4:C:140:TRP:CD2	4:C:141:PRO:HA	2.49	0.47
3:B:258:HIS:CD2	3:B:259:HIS:CD2	3.02	0.47
5:B:802:HEM:O1A	10:B:906:HOH:O	2.20	0.47
2:H:139:CYS:HB2	2:H:224:ARG:HB2	1.96	0.47
1:L:44:ASN:HB2	2:H:114:TRP:CG	2.49	0.47
3:B:309:LEU:HD12	3:B:387:MET:HG2	1.95	0.46
3:B:210:VAL:HG22	5:B:802:HEM:HMB2	1.96	0.46
3:B:239:LYS:HE2	3:B:240:TRP:HZ3	1.80	0.46
3:B:424:MET:HB3	3:B:429:THR:HG22	1.97	0.46
3:B:358:MET:HE2	3:B:358:MET:HB3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:106:VAL:HG13	4:C:109:ARG:HD3	1.97	0.46
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.98	0.46
1:L:19:ILE:HD12	1:L:19:ILE:C	2.36	0.46
3:B:258:HIS:HD2	3:B:259:HIS:CD2	2.34	0.46
2:H:98:ARG:HD3	2:H:99:SER:O	2.15	0.46
2:H:48:ILE:HG21	2:H:81:MET:CE	2.45	0.46
4:C:25:PHE:O	4:C:29:THR:CG2	2.62	0.46
3:B:239:LYS:HE2	3:B:240:TRP:CZ3	2.50	0.46
10:H:301:HOH:O	3:B:427:MET:HB2	2.14	0.46
3:B:341:THR:CG2	3:B:343:LEU:HB2	2.46	0.46
3:B:46:PHE:O	3:B:47:LEU:HB2	2.15	0.46
1:L:4:MET:HB3	1:L:99:GLY:CA	2.46	0.45
1:L:149:LYS:HD2	1:L:195:GLU:OE1	2.16	0.45
3:B:216:LEU:CD1	3:B:245:ILE:HG23	2.46	0.45
4:C:53:LYS:O	4:C:57:GLU:HG3	2.17	0.45
1:L:187:GLU:HG2	1:L:211:ARG:NH1	2.31	0.45
2:H:213:SER:O	2:H:214:SER:HB2	2.16	0.45
4:C:96:GLN:HA	4:C:96:GLN:HE21	1.82	0.45
3:B:126:ASN:ND2	3:B:132:MET:HE2	2.31	0.45
2:H:70:LEU:HD21	2:H:81:MET:HE3	1.98	0.45
3:B:203:TRP:HH2	5:B:802:HEM:HBA1	1.82	0.45
3:B:306:ALA:O	3:B:310:TRP:CD1	2.70	0.45
3:B:215:GLU:OE2	3:B:284:PHE:CZ	2.70	0.45
3:B:160:MET:O	3:B:164:ARG:HD3	2.17	0.45
3:B:426:PHE:O	3:B:430:GLN:HG2	2.16	0.45
3:B:430:GLN:NE2	4:C:110:ARG:NH1	2.65	0.45
4:C:125:LEU:HA	4:C:125:LEU:HD23	1.86	0.44
3:B:372:ARG:CG	3:B:372:ARG:NH1	2.68	0.44
4:C:82:VAL:O	4:C:87:GLY:HA2	2.18	0.44
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.50	0.44
1:L:94:TYR:C	1:L:94:TYR:CD1	2.90	0.44
4:C:77:GLU:HG3	4:C:80:ASN:ND2	2.31	0.44
3:B:305:ARG:HE	3:B:305:ARG:HB3	1.61	0.44
3:B:229:ILE:HD11	3:B:366:TYR:CD2	2.53	0.44
4:C:137:THR:HG23	4:C:140:TRP:H	1.82	0.44
3:B:353:TYR:N	5:B:801:HEM:CBC	2.80	0.44
4:C:81:VAL:HG21	9:C:201:HEC:HBA2	2.00	0.43
3:B:27:PHE:HE1	3:B:361:MET:CE	2.31	0.43
3:B:169:ALA:O	3:B:173:VAL:HG23	2.19	0.43
1:L:78:LEU:HD21	1:L:104:LEU:HD21	2.00	0.43
3:B:344:THR:HG23	5:B:802:HEM:HBD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:280:GLU:N	3:B:281:PRO:HD2	2.34	0.43
3:B:424:MET:CG	3:B:429:THR:HG22	2.49	0.43
1:L:103:LYS:HA	1:L:103:LYS:HD3	1.80	0.43
2:H:40:ARG:H	2:H:40:ARG:HG2	1.79	0.43
1:L:149:LYS:HB2	1:L:193:THR:HB	2.00	0.42
3:B:47:LEU:HD23	3:B:47:LEU:HA	1.74	0.42
2:H:199:ARG:HG2	2:H:204:ILE:HG13	2.00	0.42
3:B:304:ASN:ND2	3:B:307:VAL:HG22	2.34	0.42
3:B:197:ARG:NE	4:C:33:GLU:OE2	2.53	0.42
4:C:110:ARG:HG3	10:C:921:HOH:O	2.19	0.42
3:B:12:SER:O	3:B:15:VAL:HG22	2.19	0.42
3:B:126:ASN:CB	3:B:132:MET:CE	2.95	0.42
3:B:451:LEU:HD22	3:B:455:LEU:HD12	2.01	0.42
3:B:216:LEU:CD1	3:B:245:ILE:CG2	2.97	0.42
3:B:37:MET:HE1	3:B:60:HIS:CD2	2.55	0.42
3:B:312:MET:O	3:B:313:GLY:C	2.57	0.42
3:B:224:PHE:O	3:B:228:LYS:HG2	2.20	0.42
3:B:101:PHE:HB2	3:B:150:VAL:HG11	2.01	0.42
3:B:227:VAL:HG23	3:B:237:ILE:HG21	2.01	0.42
4:C:40:THR:O	4:C:41:ASN:HB2	2.19	0.42
3:B:53:PHE:CE1	4:C:74:PHE:HB2	2.54	0.42
3:B:52:PRO:HB2	3:B:54:ASN:ND2	2.35	0.42
3:B:346:ALA:HB2	3:B:404:LEU:HB3	2.00	0.42
3:B:268:TYR:OH	4:C:31:HIS:CD2	2.73	0.42
3:B:451:LEU:HD22	3:B:455:LEU:CD1	2.50	0.41
3:B:40:GLN:O	3:B:44:GLY:HA2	2.20	0.41
3:B:292:PHE:O	3:B:296:ASN:HB2	2.20	0.41
2:H:188:LEU:HD23	2:H:188:LEU:C	2.40	0.41
1:L:46:LEU:HD13	1:L:55:GLN:HG2	2.01	0.41
4:C:27:ALA:O	4:C:30:TYR:HB3	2.21	0.41
1:L:22:ASN:HD22	1:L:72:THR:HG22	1.85	0.41
1:L:193:THR:HG22	1:L:194:CYS:N	2.36	0.41
4:C:60:ASN:ND2	4:C:63:GLY:HA3	2.36	0.41
2:H:68:ALA:HB1	2:H:81:MET:CE	2.51	0.41
2:H:136:ALA:O	2:H:224:ARG:NH1	2.54	0.41
3:B:88:LEU:HA	3:B:161:THR:HG21	2.02	0.41
1:L:147:LYS:HB2	10:L:321:HOH:O	2.19	0.41
4:C:118:SER:O	4:C:122:VAL:HG23	2.21	0.41
4:C:77:GLU:HG3	4:C:80:ASN:HD22	1.86	0.40
4:C:99:MET:HE3	4:C:117:LEU:HD12	2.03	0.40
2:H:158:PRO:HD2	2:H:212:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ILE:O	1:L:72:THR:HA	2.21	0.40
3:B:80:VAL:HB	3:B:81:PRO:HD3	2.03	0.40
2:H:91:SER:HA	2:H:120:VAL:O	2.22	0.40
3:B:133:GLY:HA3	4:C:57:GLU:O	2.21	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	L	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	H	223/225 (99%)	210 (94%)	12 (5%)	1 (0%)	39	69
3	B	447/465 (96%)	411 (92%)	34 (8%)	2 (0%)	39	69
4	C	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
All	All	1021/1049 (97%)	955 (94%)	63 (6%)	3 (0%)	46	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	256	THR
3	B	380	ASN
2	H	196	SER

### 5.3.2 Protein sidechains [i](#)

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	L	189/189 (100%)	164 (87%)	25 (13%)	5	12
2	H	192/192 (100%)	158 (82%)	34 (18%)	2	5
3	B	360/371 (97%)	304 (84%)	56 (16%)	3	8
4	C	116/120 (97%)	105 (90%)	11 (10%)	11	24
All	All	857/872 (98%)	731 (85%)	126 (15%)	4	9

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	3	GLN
1	L	4	MET
1	L	7	SER
1	L	20	THR
1	L	24	ARG
1	L	27	LYS
1	L	43	THR
1	L	46	LEU
1	L	54	LEU
1	L	55	GLN
1	L	65	SER
1	L	69	THR
1	L	79	GLU
1	L	90	GLN
1	L	94	TYR
1	L	96	LEU
1	L	103	LYS
1	L	106	LEU
1	L	142	LYS
1	L	169	LYS
1	L	171	SER
1	L	179	LEU
1	L	197	THR
1	L	213	GLU
2	H	5	GLN
2	H	7	SER
2	H	10	VAL
2	H	11	LEU
2	H	17	SER
2	H	18	VAL

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Mol	Chain	Res	Type
2	H	23	LYS
2	H	30	THR
2	H	34	MET
2	H	40	ARG
2	H	43	GLN
2	H	65	LYS
2	H	78	THR
2	H	87	THR
2	H	98	ARG
2	H	106	VAL
2	H	111	PHE
2	H	126	LYS
2	H	135	LEU
2	H	139	CYS
2	H	142	THR
2	H	143	THR
2	H	147	VAL
2	H	148	THR
2	H	152	LEU
2	H	160	PRO
2	H	170	LEU
2	H	187	THR
2	H	188	LEU
2	H	189	SER
2	H	192	VAL
2	H	194	VAL
2	H	199	ARG
2	H	219	LYS
3	B	39	LEU
3	B	54	ASN
3	B	64	LEU
3	B	67	TRP
3	B	79	LEU
3	B	92	LYS
3	B	93	LEU
3	B	96	ILE
3	B	107	LEU
3	B	108	THR
3	B	115	VAL
3	B	127	GLU
3	B	139	GLN
3	B	164	ARG

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Mol	Chain	Res	Type
3	B	174	LEU
3	B	195	LEU
3	B	196	THR
3	B	210	VAL
3	B	213	VAL
3	B	222	LEU
3	B	240	TRP
3	B	241	LEU
3	B	245	ILE
3	B	258	HIS
3	B	283	PRO
3	B	288	VAL
3	B	296	ASN
3	B	297	ARG
3	B	298	ARG
3	B	300	ARG
3	B	305	ARG
3	B	307	VAL
3	B	309	LEU
3	B	328	MET
3	B	329	HIS
3	B	341	THR
3	B	343	LEU
3	B	352	PHE
3	B	358	MET
3	B	363	ILE
3	B	372	ARG
3	B	381	ARG
3	B	385	LEU
3	B	387	MET
3	B	401	THR
3	B	404	LEU
3	B	410	LEU
3	B	413	TRP
3	B	416	ARG
3	B	427	MET
3	B	429	THR
3	B	433	LEU
3	B	435	ILE
3	B	440	ARG
3	B	448	LEU
3	B	451	LEU

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Mol	Chain	Res	Type
4	C	9	MET
4	C	24	LEU
4	C	29	THR
4	C	33	GLU
4	C	38	GLU
4	C	67	LEU
4	C	80	ASN
4	C	95	LEU
4	C	106	VAL
4	C	137	THR
4	C	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	22	ASN
1	L	89	GLN
1	L	91	HIS
1	L	137	ASN
1	L	161	ASN
1	L	198	HIS
2	H	175	HIS
2	H	182	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	126	ASN
3	B	139	GLN
3	B	296	ASN
3	B	329	HIS
3	B	411	GLN
3	B	430	GLN
4	C	31	HIS
4	C	60	ASN
4	C	80	ASN
4	C	96	GLN
4	C	102	GLN
4	C	105	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 ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
5	HEM	B	801	8,3	30,50,50	2.24	7 (23%)	24,82,82	3.18	13 (54%)
5	HEM	B	802	8,3,7	30,50,50	2.34	5 (16%)	24,82,82	2.82	9 (37%)
9	HEC	C	201	4	24,50,50	2.62	4 (16%)	19,82,82	3.19	7 (36%)

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
5	HEM	B	801	8,3	-	0/10/54/54	0/0/8/8
5	HEM	B	802	8,3,7	-	0/10/54/54	0/0/8/8
9	HEC	C	201	4	-	0/6/54/54	0/0/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	HEM	C3B-C4B	-9.08	1.43	1.51
9	C	201	HEC	C3B-C2B	-8.02	1.32	1.40
5	B	801	HEM	C3B-C4B	-7.32	1.45	1.51
9	C	201	HEC	C3C-C2C	-7.30	1.33	1.40
5	B	801	HEM	C3D-C4D	-5.29	1.44	1.51
5	B	802	HEM	C3D-C4D	-4.89	1.45	1.51
5	B	802	HEM	C2C-C1C	-4.40	1.44	1.52
5	B	801	HEM	C2C-C1C	-4.31	1.44	1.52
5	B	802	HEM	C2D-C1D	-2.38	1.44	1.51
5	B	801	HEM	C2B-C1B	-2.13	1.44	1.51
5	B	801	HEM	C2D-C1D	-2.08	1.45	1.51
5	B	802	HEM	FE-ND	2.18	2.09	1.97
9	C	201	HEC	C3B-C4B	2.41	1.48	1.42
5	B	801	HEM	C1C-NC	2.48	1.39	1.36
5	B	801	HEM	FE-NC	4.33	2.12	1.95
9	C	201	HEC	C3D-C2D	5.00	1.52	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	HEM	CBA-CAA-C2A	-8.13	97.96	112.53
9	C	201	HEC	CBC-CAC-C3C	-7.15	111.46	127.35
5	B	801	HEM	C3C-CAC-CBC	-7.02	113.68	124.46
5	B	801	HEM	C3B-CAB-CBB	-6.94	113.80	124.46
9	C	201	HEC	CBD-CAD-C3D	-6.62	100.67	112.53
9	C	201	HEC	CBB-CAB-C3B	-5.97	114.09	127.35
9	C	201	HEC	CBA-CAA-C2A	-4.64	104.21	112.53
9	C	201	HEC	CAA-C2A-C1A	-3.75	122.93	127.01
5	B	801	HEM	C3B-C4B-NB	-3.40	105.13	111.63
5	B	801	HEM	C4B-CHC-C1C	-2.89	121.00	125.82
5	B	802	HEM	CAA-CBA-CGA	-2.79	107.64	112.75
9	C	201	HEC	CMB-C2B-C1B	-2.48	124.26	128.36
5	B	801	HEM	CBD-CAD-C3D	-2.40	106.58	113.55
5	B	802	HEM	C3C-CAC-CBC	-2.10	121.23	124.46
5	B	802	HEM	CAA-C2A-C1A	-2.05	124.78	127.01
5	B	801	HEM	CBA-CAA-C2A	2.03	116.18	112.53
5	B	801	HEM	CMD-C2D-C3D	2.30	124.51	114.35
9	C	201	HEC	CMA-C3A-C2A	2.37	130.20	125.24
5	B	801	HEM	CMC-C2C-C3C	2.58	122.98	116.53
5	B	801	HEM	CHC-C4B-NB	2.68	130.97	124.52
5	B	802	HEM	CMD-C2D-C3D	2.93	127.33	114.35
5	B	801	HEM	CMB-C2B-C3B	3.17	124.46	116.53
5	B	801	HEM	CAD-C3D-C2D	4.21	125.32	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	HEM	CMB-C2B-C3B	4.33	127.33	116.53
5	B	802	HEM	CAD-C3D-C2D	4.59	126.42	113.22
5	B	802	HEM	CMC-C2C-C3C	4.80	128.51	116.53
5	B	801	HEM	C2C-C1C-CHC	4.84	131.04	123.68
5	B	802	HEM	CAD-C3D-C4D	5.10	130.47	112.47
5	B	801	HEM	CAD-C3D-C4D	5.26	131.02	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	HEM	3	0
5	B	802	HEM	5	0
9	C	201	HEC	6	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	L	213/213 (100%)	-0.47	1 (0%) 91 93	48, 72, 99, 121	1 (0%)
2	H	225/225 (100%)	-0.23	13 (5%) 26 25	48, 70, 107, 134	3 (1%)
3	B	449/465 (96%)	-0.30	24 (5%) 30 28	57, 89, 141, 179	0
4	C	142/146 (97%)	-0.46	4 (2%) 56 57	49, 78, 114, 137	0
All	All	1029/1049 (98%)	-0.34	42 (4%) 41 41	48, 79, 129, 179	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	225	GLY	6.9
3	B	381	ARG	4.8
2	H	141	ASP	4.3
4	C	139	GLN	4.1
3	B	85	ASP	4.0
2	H	206	CYS	4.0
3	B	299	ARG	3.8
3	B	77	TYR	3.7
3	B	373	GLY	3.5
3	B	374	ILE	3.4
3	B	297	ARG	3.4
2	H	143	THR	3.2
3	B	164	ARG	3.1
4	C	5	PHE	3.1
2	H	202	GLN	3.0
2	H	151	CYS	2.9
3	B	95	TRP	2.8
3	B	435	ILE	2.7
3	B	86	CYS	2.7
2	H	41	PRO	2.7
2	H	22	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	16	ALA	2.5
3	B	128	LEU	2.4
1	L	126	THR	2.4
3	B	292	PHE	2.4
3	B	233	ASP	2.3
3	B	129	TRP	2.3
3	B	384	VAL	2.3
3	B	375	GLY	2.3
2	H	150	GLY	2.3
3	B	96	ILE	2.2
2	H	42	GLY	2.2
3	B	296	ASN	2.2
3	B	80	VAL	2.2
4	C	89	GLU	2.2
2	H	116	GLN	2.1
2	H	183	SER	2.1
2	H	43	GLN	2.1
3	B	99	TRP	2.1
3	B	127	GLU	2.1
3	B	76	ALA	2.1
4	C	30	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
9	HEC	C	201	43/43	0.99	0.14	0.61	50,58,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HEM	B	801	43/43	0.99	0.14	0.37	51,59,68,76	0
5	HEM	B	802	43/43	0.99	0.13	0.24	57,66,73,83	0
7	O	B	805	1/1	1.00	0.15	-0.12	60,60,60,60	0
8	CA	C	804	1/1	0.98	0.04	-4.71	60,60,60,60	0
6	FE	B	803	1/1	1.00	0.12	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.