



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 PM GMT

PDB ID : 4HGI  
Title : Crystal structure of P450 BM3 5F5 heme domain variant complexed with styrene (dataset II)  
Authors : Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.  
Deposited on : 2012-10-08  
Resolution : 1.50 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

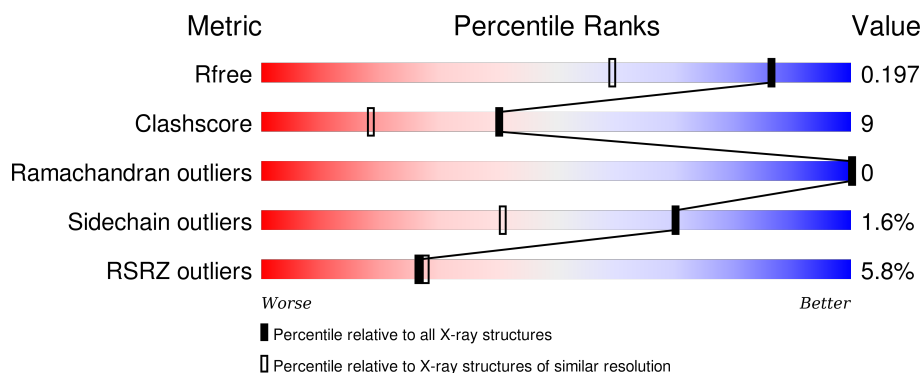
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	455	<div> <div>5%</div> <div>88%</div> <div>12%</div> </div>
1	B	455	<div> <div>6%</div> <div>84%</div> <div>14%</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
3	SYN	A	502[A]	-	-	X	X
3	SYN	A	502[B]	-	-	-	X
3	SYN	B	503[A]	-	-	X	X
3	SYN	B	503[B]	-	-	-	X
4	GOL	A	503	-	-	-	X
4	GOL	B	501	-	-	-	X
4	GOL	B	504	-	-	-	X
5	PEG	A	505	-	-	X	X
6	MES	B	505	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8715 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.

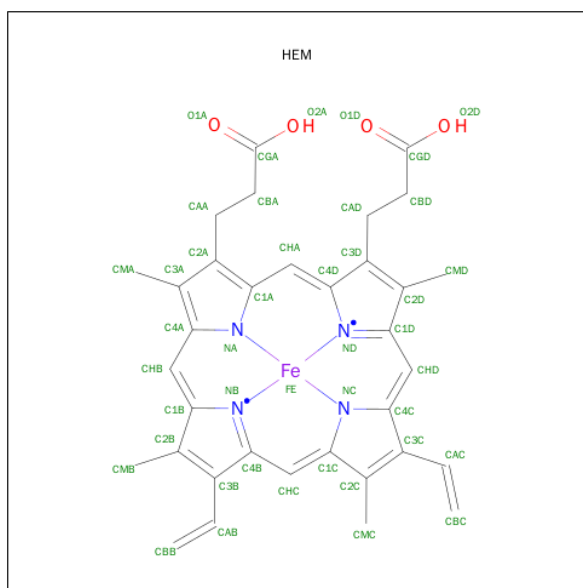
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	31	0
			3824	2461	635	707	21			
1	B	453	Total	C	N	O	S	0	31	0
			3808	2454	631	704	19			

There are 4 discrepancies between the modelled and reference sequences:

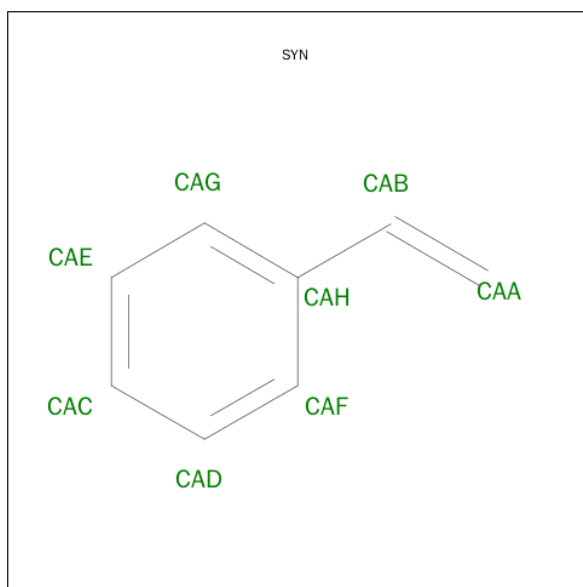
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
A	235	ALA	THR	ENGINEERED MUTATION	UNP P14779
B	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
B	235	ALA	THR	ENGINEERED MUTATION	UNP P14779

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ETHENYLBENZENE (three-letter code: SYN) (formula:  $C_8H_8$ ).



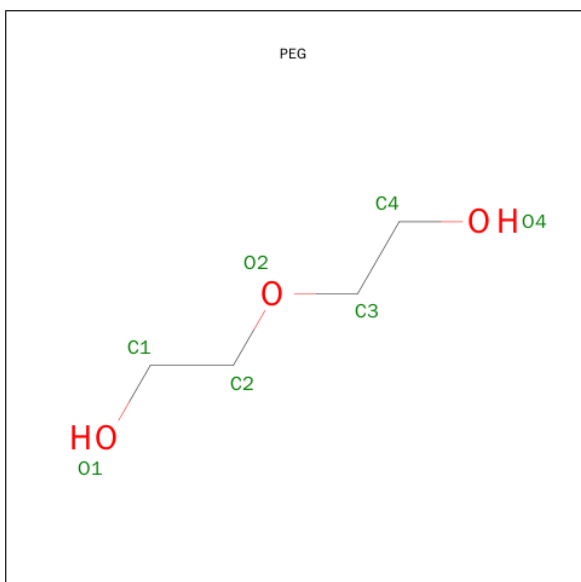
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	1
			16	16		
3	B	1	Total	C	0	1
			16	16		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



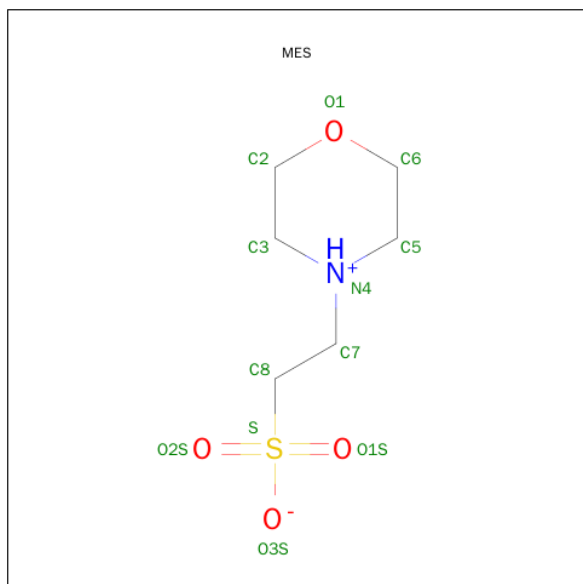
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

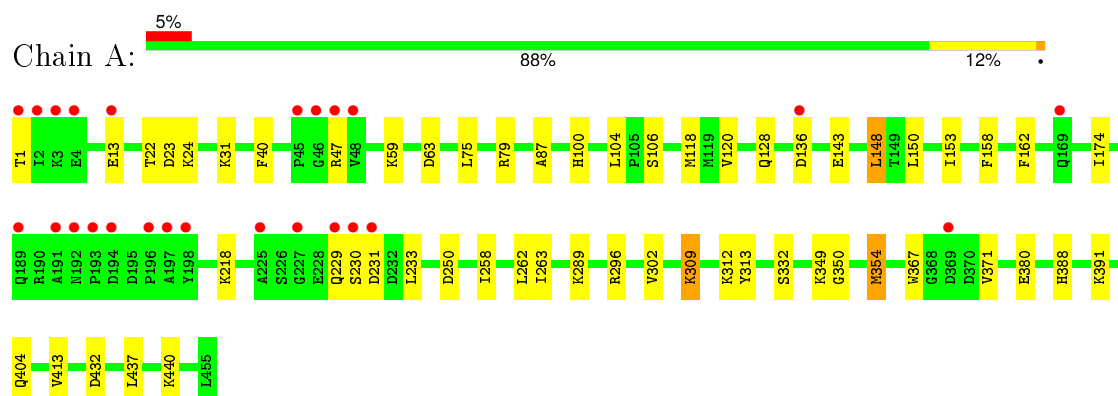
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	489	Total	O	0	2
			489	489		
7	B	427	Total	O	0	0
			427	427		

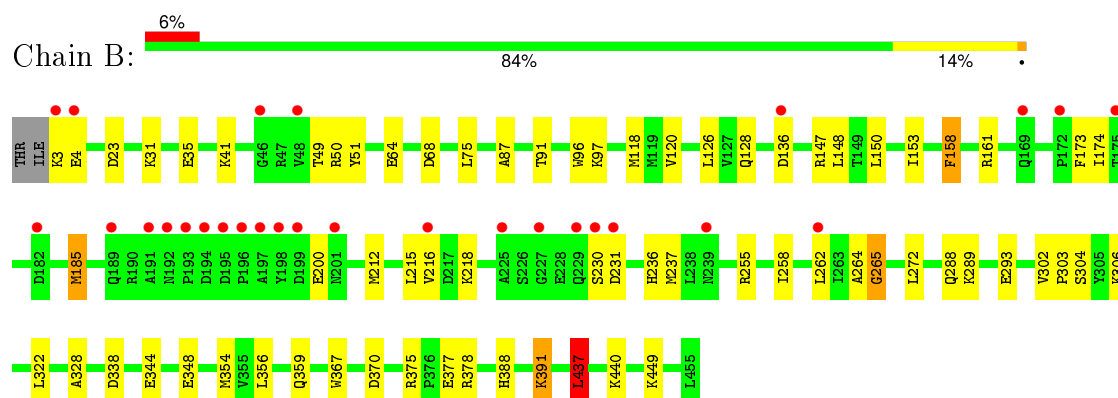
### 3 Residue-property plots [i](#)

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: Bifunctional P-450/NADPH-P450 reductase



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.99 Å   148.89 Å   64.82 Å 90.00°   98.37°   90.00°	Depositor
Resolution (Å)	19.99 – 1.50 19.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	88.5 (19.99-1.50) 88.5 (19.98-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.50 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.178   ,   0.199 0.176   ,   0.197	Depositor DCC
$R_{free}$ test set	959 reflections (0.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 155737 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, SYN, MES, 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	1.22	3/3998 (0.1%)	1.04	9/5398 (0.2%)
1	B	1.18	7/3983 (0.2%)	1.07	13/5378 (0.2%)
All	All	1.20	10/7981 (0.1%)	1.05	22/10776 (0.2%)

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	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CD-OE1	-7.57	1.17	1.25
1	B	64	GLU	CD-OE2	-5.88	1.19	1.25
1	B	367	TRP	CD2-CE2	5.84	1.48	1.41
1	B	348	GLU	CD-OE2	-5.81	1.19	1.25
1	A	40	PHE	CG-CD2	5.35	1.46	1.38
1	B	96	TRP	CD2-CE2	5.32	1.47	1.41
1	B	293	GLU	CD-OE2	5.31	1.31	1.25
1	B	377	GLU	CD-OE1	5.24	1.31	1.25
1	B	304	SER	CB-OG	5.06	1.48	1.42
1	A	380	GLU	C-O	5.03	1.32	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CB-CG-OD1	7.32	124.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	161	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	250	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	437	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	147	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	354[A]	MET	CG-SD-CE	5.69	109.31	100.20
1	A	354[B]	MET	CG-SD-CE	5.69	109.31	100.20
1	B	147	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	432	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	378	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	79	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	59[A]	LYS	CD-CE-NZ	5.45	124.24	111.70
1	A	59[B]	LYS	CD-CE-NZ	5.45	124.24	111.70
1	B	237	MET	CG-SD-CE	5.45	108.92	100.20
1	B	158[A]	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	B	158[B]	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	A	63	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	391[A]	LYS	CD-CE-NZ	5.22	123.71	111.70
1	B	391[B]	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	309	LYS	CD-CE-NZ	5.15	123.56	111.70
1	B	96	TRP	CA-CB-CG	-5.05	104.10	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	265[A]	GLY	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	3824	0	3900	60	0
1	B	3808	0	3878	77	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	16	0	16	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	16	11	0
4	A	18	0	24	1	0
4	B	12	0	15	2	0
5	A	7	0	10	6	0
6	B	12	0	12	1	0
7	A	489	0	0	9	0
7	B	427	0	0	14	0
All	All	8715	0	7931	137	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 9.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150[A]:LEU:HD21	1:B:174:ILE:CD1	1.23	1.66
1:B:150[A]:LEU:CD2	1:B:174:ILE:CD1	1.96	1.43
1:B:158[A]:PHE:CE1	1:B:258:ILE:HG12	1.62	1.34
1:A:289[B]:LYS:CB	1:A:289[B]:LYS:NZ	1.79	1.31
1:B:150[A]:LEU:CD2	1:B:174:ILE:HD13	1.60	1.28
1:A:289[B]:LYS:CB	1:A:289[B]:LYS:HZ3	1.21	1.23
1:B:370:ASP:OD2	1:B:375:ARG:NH1	1.74	1.21
1:B:264:ALA:O	3:B:503[A]:SYN:CAA	1.91	1.18
1:A:289[B]:LYS:HB3	1:A:289[B]:LYS:NZ	0.91	1.15
1:A:22[B]:THR:HG22	1:A:24:LYS:H	1.17	1.10
1:B:212:MET:O	1:B:216[B]:VAL:HG23	1.55	1.07
1:B:150[A]:LEU:CD2	1:B:174:ILE:HD11	1.72	0.97
1:B:158[A]:PHE:HE1	1:B:258:ILE:HG12	1.23	0.95
1:B:150[A]:LEU:HD21	1:B:174:ILE:CG1	1.98	0.92
1:B:440:LYS:HD3	7:B:995:HOH:O	1.70	0.91
1:B:150[A]:LEU:HD21	1:B:174:ILE:HD11	0.91	0.89
1:B:264:ALA:O	3:B:503[A]:SYN:H9	1.72	0.89
1:A:87:ALA:HB1	3:A:502[A]:SYN:H4	1.57	0.87
1:A:22[B]:THR:HG22	1:A:24:LYS:N	1.92	0.83
1:B:118[B]:MET:SD	7:B:799:HOH:O	2.36	0.83
1:A:349:LYS:HG2	5:A:505:PEG:H32	1.59	0.82
1:A:289[B]:LYS:HB3	1:A:289[B]:LYS:HZ2	0.94	0.77
1:B:158[A]:PHE:CE1	1:B:258:ILE:CG1	2.58	0.76
1:B:264:ALA:HB1	3:B:503[A]:SYN:H8	1.66	0.76
1:B:356[A]:LEU:HD23	1:B:359[A]:GLN:HG3	1.67	0.76
1:B:264:ALA:O	3:B:503[A]:SYN:H8	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[B]:THR:CG2	1:A:24:LYS:H	1.96	0.75
1:B:150[A]:LEU:HD23	1:B:174:ILE:HD13	1.66	0.74
1:B:150[A]:LEU:HD22	1:B:174:ILE:HD13	1.66	0.73
1:A:148[B]:LEU:HD11	1:A:413:VAL:HG21	1.69	0.73
1:B:49[A]:THR:CG2	1:B:354[A]:MET:HG2	2.19	0.73
1:B:49[A]:THR:HG21	1:B:354[A]:MET:HG2	1.72	0.72
1:A:289[B]:LYS:HE3	1:A:313:TYR:CZ	2.25	0.71
1:B:288[B]:GLN:OE1	7:B:753:HOH:O	2.08	0.71
1:A:332:SER:HB2	1:A:354[B]:MET:CE	2.21	0.71
1:A:75:LEU:HD21	3:A:502[A]:SYN:H3	1.71	0.70
1:B:23:ASP:OD2	7:B:976:HOH:O	2.10	0.69
1:B:150[A]:LEU:HD23	1:B:174:ILE:CD1	2.18	0.69
1:A:158:PHE:CD1	1:A:258[A]:ILE:HD12	2.28	0.69
1:B:264:ALA:HB1	3:B:503[A]:SYN:H5	1.74	0.69
1:B:185:MET:HE1	1:B:437:LEU:HD23	1.74	0.68
1:B:158[B]:PHE:CZ	1:B:262[B]:LEU:HD21	2.30	0.66
1:A:349:LYS:HE2	5:A:505:PEG:H21	1.77	0.66
1:A:230[A]:SER:OG	1:A:231:ASP:N	2.29	0.64
1:A:263:ILE:HG22	3:A:502[B]:SYN:H6	1.79	0.64
1:A:153[B]:ILE:HG23	1:A:262:LEU:HD23	1.80	0.63
1:A:136:ASP:OD1	1:B:218:LYS:CE	2.47	0.63
1:A:440:LYS:HE2	7:A:970:HOH:O	1.99	0.63
1:A:296[B]:ARG:NH2	7:A:975:HOH:O	2.34	0.61
1:B:236:HIS:CE1	7:B:921:HOH:O	2.53	0.61
1:B:153[B]:ILE:HG13	7:B:809:HOH:O	1.99	0.61
1:A:332:SER:HB2	1:A:354[B]:MET:HE2	1.83	0.59
1:A:153[A]:ILE:HG13	7:A:964:HOH:O	2.01	0.59
1:B:185:MET:CE	1:B:437:LEU:HD23	2.33	0.59
1:A:289[B]:LYS:CA	1:A:289[B]:LYS:HZ3	2.10	0.58
1:A:120:VAL:HG11	1:A:302[A]:VAL:HG13	1.84	0.58
1:B:3:LYS:HG3	1:B:344:GLU:OE2	2.05	0.56
1:B:264:ALA:C	3:B:503[A]:SYN:H8	2.25	0.56
1:B:264:ALA:CB	3:B:503[A]:SYN:H8	2.34	0.56
1:B:388:HIS:ND1	1:B:391[B]:LYS:HE3	2.21	0.56
1:A:75:LEU:HD21	3:A:502[A]:SYN:CAC	2.35	0.55
1:B:4:GLU:OE2	1:B:4:GLU:N	2.36	0.55
1:B:49[A]:THR:HG21	1:B:354[A]:MET:CG	2.35	0.55
1:B:288[B]:GLN:CD	7:B:753:HOH:O	2.45	0.54
1:A:437:LEU:HD23	7:A:1044:HOH:O	2.08	0.54
1:A:349:LYS:CG	5:A:505:PEG:H32	2.37	0.54
1:A:136:ASP:OD1	1:B:218:LYS:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:HE1	4:A:506:GOL:O2	1.91	0.54
1:B:158[B]:PHE:HZ	1:B:262[B]:LEU:HD21	1.72	0.52
1:B:158[A]:PHE:HE1	1:B:258:ILE:CG1	2.10	0.52
1:B:153[A]:ILE:CG2	1:B:262[A]:LEU:HD23	2.40	0.52
1:A:128[A]:GLN:NE2	7:A:961:HOH:O	2.42	0.52
1:B:264:ALA:CA	3:B:503[A]:SYN:H8	2.40	0.52
1:B:158[B]:PHE:CE1	1:B:262[B]:LEU:HD21	2.44	0.51
1:A:309:LYS:O	1:A:312:LYS:HE3	2.11	0.51
1:B:265[A]:GLY:HA3	2:B:502:HEM:C2C	2.47	0.50
1:B:173:PHE:CE2	1:B:262[B]:LEU:HD13	2.46	0.50
1:B:158[A]:PHE:CZ	1:B:258:ILE:HG12	2.36	0.50
1:A:150[B]:LEU:CD1	1:A:162:PHE:CD2	2.95	0.50
1:B:68:ASP:CG	4:B:504:GOL:H32	2.33	0.50
1:B:153[A]:ILE:HG23	1:B:262[A]:LEU:HD23	1.95	0.48
1:B:87:ALA:HB1	3:B:503[A]:SYN:H4	1.96	0.48
1:A:120:VAL:HG11	1:A:302[A]:VAL:CG1	2.43	0.48
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.48
1:A:23[B]:ASP:HB3	1:A:24:LYS:HG3	1.95	0.47
1:A:349:LYS:HG2	5:A:505:PEG:H21	1.95	0.47
1:B:328:ALA:HB2	3:B:503[B]:SYN:H3	1.97	0.47
1:B:35[A]:GLU:HG3	7:B:1007:HOH:O	2.15	0.46
1:A:118[B]:MET:HE1	7:A:806:HOH:O	2.14	0.46
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.97	0.46
1:B:288[B]:GLN:HA	1:B:288[B]:GLN:NE2	2.31	0.46
1:A:153[B]:ILE:CG2	1:A:262:LEU:HD23	2.46	0.46
1:B:216[B]:VAL:HG11	1:B:255:ARG:HG2	1.97	0.46
1:B:288[B]:GLN:NE2	7:B:753:HOH:O	2.49	0.46
1:A:218:LYS:HE3	1:B:136:ASP:OD2	2.16	0.46
1:A:350:GLY:CA	5:A:505:PEG:H12	2.46	0.45
1:B:153[A]:ILE:HG23	1:B:262[A]:LEU:CD2	2.47	0.45
1:A:100:HIS:NE2	1:A:104[B]:LEU:HD11	2.32	0.44
1:A:350:GLY:HA2	5:A:505:PEG:H12	1.99	0.44
6:B:505:MES:H51	7:B:684:HOH:O	2.18	0.44
1:B:75:LEU:HD21	3:B:503[A]:SYN:H3	1.98	0.44
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.99	0.44
1:A:150[B]:LEU:CD1	1:A:174:ILE:HD11	2.48	0.43
1:B:200:GLU:HA	1:B:200:GLU:OE1	2.16	0.43
1:B:216[B]:VAL:HG11	1:B:255:ARG:CG	2.48	0.43
1:B:303:PRO:HG3	7:B:928:HOH:O	2.18	0.43
1:B:150[A]:LEU:HD21	1:B:174:ILE:HG12	1.91	0.43
1:B:128[A]:GLN:NE2	7:B:938:HOH:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LYS:HE3	7:B:763:HOH:O	2.18	0.43
1:A:148[A]:LEU:HD21	1:A:413:VAL:HG21	1.99	0.43
1:B:289[A]:LYS:HG3	7:B:821:HOH:O	2.19	0.42
1:B:150[A]:LEU:CD2	1:B:174:ILE:CG1	2.76	0.42
1:B:173:PHE:HB2	1:B:215:LEU:HD22	2.01	0.42
1:B:354[B]:MET:HE3	1:B:354[B]:MET:HB2	1.75	0.42
1:A:31[A]:LYS:HG3	7:A:747:HOH:O	2.20	0.42
1:A:404[B]:GLN:NE2	7:A:967:HOH:O	2.50	0.42
3:A:502[A]:SYN:H1	7:A:1043:HOH:O	2.19	0.42
1:A:106[A]:SER:HB3	1:A:233:LEU:HD23	2.02	0.42
1:A:87:ALA:HB1	3:A:502[A]:SYN:CAE	2.39	0.42
1:A:388:HIS:HA	1:A:391:LYS:HD3	2.02	0.41
1:A:150[B]:LEU:HG	1:A:174:ILE:CD1	2.51	0.41
1:A:104[B]:LEU:HA	1:A:104[B]:LEU:HD23	1.95	0.41
3:A:502[B]:SYN:H5	3:A:502[B]:SYN:H8	1.79	0.41
1:A:100:HIS:CE1	1:A:104[B]:LEU:HD11	2.56	0.41
1:A:263:ILE:HG21	1:A:263:ILE:HD13	1.83	0.41
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.37	0.41
1:A:120:VAL:CG1	1:A:302[B]:VAL:CG2	2.98	0.41
1:B:185:MET:HE2	1:B:437:LEU:HA	2.02	0.40
1:B:91:THR:CG2	4:B:504:GOL:H2	2.51	0.40
1:B:97[B]:LYS:HA	1:B:97[B]:LYS:HD2	1.85	0.40
1:B:51:TYR:CE2	1:B:354[B]:MET:HG2	2.56	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	484/455 (106%)	467 (96%)	17 (4%)	0	100	100
1	B	482/455 (106%)	469 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	966/910 (106%)	936 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	427/397 (108%)	421 (99%)	6 (1%)	74	47
1	B	425/397 (107%)	416 (98%)	9 (2%)	61	27
All	All	852/794 (107%)	837 (98%)	15 (2%)	70	35

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	13	GLU
1	A	47	ARG
1	A	148[A]	LEU
1	A	148[B]	LEU
1	A	229	GLN
1	B	31	LYS
1	B	41	LYS
1	B	148	LEU
1	B	185	MET
1	B	230[A]	SER
1	B	230[B]	SER
1	B	231	ASP
1	B	437	LEU
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	21	ASN
1	A	189	GLN
1	A	206	GLN
1	B	201	ASN
1	B	204	GLN

### 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 ⓘ

13 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	1,7	30,50,50	2.59	8 (26%)	24,82,82	2.64	11 (45%)
3	SYN	A	502[A]	-	8,8,8	1.57	2 (25%)	9,9,9	1.09	1 (11%)
3	SYN	A	502[B]	-	8,8,8	1.72	2 (25%)	9,9,9	1.29	2 (22%)
4	GOL	A	503	-	5,5,5	0.58	0	5,5,5	1.78	2 (40%)
4	GOL	A	504	-	5,5,5	0.50	0	5,5,5	1.19	0
5	PEG	A	505	-	6,6,6	1.01	0	5,5,5	1.60	1 (20%)
4	GOL	A	506	-	5,5,5	0.92	0	5,5,5	0.97	0
4	GOL	B	501	-	5,5,5	0.44	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	502	1,7	30,50,50	2.77	7 (23%)	24,82,82	2.74	13 (54%)
3	SYN	B	503[A]	-	8,8,8	1.76	2 (25%)	9,9,9	1.28	1 (11%)
3	SYN	B	503[B]	-	8,8,8	1.50	2 (25%)	9,9,9	0.73	0
4	GOL	B	504	-	5,5,5	1.00	0	5,5,5	1.25	0
6	MES	B	505	-	11,12,12	0.60	0	14,16,16	8.77	8 (57%)

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	1,7	-	0/10/54/54	0/0/8/8
3	SYN	A	502[A]	-	-	0/2/2/2	0/1/1/1
3	SYN	A	502[B]	-	-	0/2/2/2	0/1/1/1
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
4	GOL	A	504	-	-	0/4/4/4	0/0/0/0
5	PEG	A	505	-	-	0/4/4/4	0/0/0/0
4	GOL	A	506	-	-	0/4/4/4	0/0/0/0
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	HEM	B	502	1,7	-	0/10/54/54	0/0/8/8
3	SYN	B	503[A]	-	-	0/2/2/2	0/1/1/1
3	SYN	B	503[B]	-	-	0/2/2/2	0/1/1/1
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
6	MES	B	505	-	-	0/6/14/14	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	C3B-C4B	-10.29	1.42	1.51
2	A	501	HEM	C3B-C4B	-9.28	1.43	1.51
2	B	502	HEM	C3D-C4D	-5.99	1.43	1.51
2	A	501	HEM	C3D-C4D	-5.76	1.44	1.51
2	B	502	HEM	C2C-C1C	-4.66	1.43	1.52
2	A	501	HEM	C2C-C1C	-4.26	1.44	1.52
3	B	503[A]	SYN	CAH-CAB	-3.44	1.36	1.49
3	A	502[B]	SYN	CAH-CAB	-3.10	1.37	1.49
2	A	501	HEM	C2D-C1D	-2.90	1.42	1.51
2	A	501	HEM	C2B-C1B	-2.77	1.42	1.51
2	B	502	HEM	C2D-C1D	-2.66	1.43	1.51
3	A	502[A]	SYN	CAH-CAB	-2.56	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503[B]	SYN	CAH-CAB	-2.41	1.40	1.49
2	B	502	HEM	C2B-C1B	-2.37	1.44	1.51
2	A	501	HEM	CAA-C2A	2.65	1.56	1.52
3	B	503[B]	SYN	CAA-CAB	3.01	1.50	1.28
3	A	502[B]	SYN	CAA-CAB	3.18	1.51	1.28
2	A	501	HEM	FE-ND	3.27	2.14	1.97
3	B	503[A]	SYN	CAA-CAB	3.29	1.52	1.28
3	A	502[A]	SYN	CAA-CAB	3.33	1.53	1.28
2	B	502	HEM	FE-NB	3.70	2.17	1.97
2	A	501	HEM	FE-NC	3.71	2.10	1.95
2	B	502	HEM	FE-NC	4.49	2.13	1.95

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	505	MES	O1S-S-C8	-27.51	83.43	106.91
6	B	505	MES	O2S-S-C8	-14.53	94.51	106.91
2	A	501	HEM	CMA-C3A-C4A	-3.89	121.94	128.36
6	B	505	MES	C2-C3-N4	-3.81	104.35	110.12
2	B	502	HEM	C3B-C4B-NB	-3.48	104.98	111.63
2	A	501	HEM	C3B-C4B-NB	-3.47	105.00	111.63
2	B	502	HEM	CAA-C2A-C1A	-3.37	123.35	127.01
4	A	503	GOL	O3-C3-C2	-2.68	97.17	110.18
2	A	501	HEM	C2C-C1C-NC	-2.68	105.69	110.21
2	B	502	HEM	CMA-C3A-C4A	-2.64	124.00	128.36
4	A	503	GOL	O1-C1-C2	-2.50	98.08	110.18
2	B	502	HEM	C2C-C1C-NC	-2.12	106.63	110.21
3	A	502[B]	SYN	CAH-CAB-CAA	-2.12	113.05	125.94
3	A	502[A]	SYN	CAH-CAB-CAA	-2.02	113.66	125.94
2	B	502	HEM	CHD-C1D-ND	2.06	129.48	124.52
3	A	502[B]	SYN	CAF-CAH-CAG	2.15	120.92	117.64
5	A	505	PEG	O2-C3-C4	2.20	120.58	110.43
6	B	505	MES	C7-N4-C5	2.22	116.95	111.27
2	B	502	HEM	CMD-C2D-C3D	2.41	124.99	114.35
3	B	503[A]	SYN	CAF-CAH-CAG	2.46	121.40	117.64
6	B	505	MES	O3S-S-O2S	2.52	117.47	111.61
2	A	501	HEM	C2C-C1C-CHC	2.52	127.52	123.68
2	A	501	HEM	C2D-C3D-C4D	2.53	105.80	101.50
2	A	501	HEM	CMD-C2D-C3D	2.75	126.53	114.35
2	B	502	HEM	C2D-C3D-C4D	2.94	106.48	101.50
2	B	502	HEM	CAA-CBA-CGA	3.08	118.40	112.75
2	A	501	HEM	C3B-C4B-CHC	3.43	128.00	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CAD-C3D-C2D	3.70	123.86	113.22
2	B	502	HEM	C3B-C4B-CHC	4.07	128.89	123.16
6	B	505	MES	C7-N4-C3	4.10	121.78	111.27
2	B	502	HEM	CAD-C3D-C4D	4.15	127.10	112.47
2	B	502	HEM	CAD-C3D-C2D	4.58	126.40	113.22
2	A	501	HEM	CMC-C2C-C3C	4.72	128.31	116.53
2	A	501	HEM	CMB-C2B-C3B	4.76	128.41	116.53
6	B	505	MES	O3S-S-O1S	5.05	123.36	111.61
2	A	501	HEM	CAD-C3D-C4D	5.07	130.34	112.47
2	B	502	HEM	CMB-C2B-C3B	5.07	129.19	116.53
2	B	502	HEM	CMC-C2C-C3C	5.32	129.81	116.53
6	B	505	MES	C5-N4-C3	5.71	121.26	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[A]	SYN	5	0
3	A	502[B]	SYN	2	0
5	A	505	PEG	6	0
4	A	506	GOL	1	0
2	B	502	HEM	1	0
3	B	503[A]	SYN	10	0
3	B	503[B]	SYN	1	0
4	B	504	GOL	2	0
6	B	505	MES	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	455/455 (100%)	0.12	25 (5%)	29 30	8, 15, 33, 95	0
1	B	453/455 (99%)	0.34	28 (6%)	24 25	8, 16, 51, 128	0
All	All	908/910 (99%)	0.23	53 (5%)	26 28	8, 15, 41, 128	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	PRO	9.0
1	B	191	ALA	9.0
1	B	197	ALA	7.9
1	A	1	THR	7.3
1	B	192	ASN	7.0
1	B	225	ALA	5.9
1	B	198	TYR	5.8
1	B	4	GLU	5.7
1	B	194	ASP	5.2
1	B	231	ASP	5.0
1	A	191	ALA	4.7
1	B	193	PRO	4.4
1	B	199	ASP	4.4
1	A	2	ILE	4.3
1	B	195	ASP	3.7
1	A	229	GLN	3.6
1	A	46	GLY	3.5
1	B	46	GLY	3.5
1	B	169	GLN	3.4
1	B	189	GLN	3.4
1	B	227	GLY	3.3
1	A	169	GLN	3.2
1	B	3	LYS	3.2
1	A	230[A]	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLN	3.1
1	A	4	GLU	3.0
1	B	182	ASP	3.0
1	A	192	ASN	3.0
1	B	239	ASN	2.9
1	B	175	THR	2.9
1	A	194	ASP	2.9
1	A	231	ASP	2.9
1	A	48	VAL	2.8
1	A	3	LYS	2.8
1	A	13	GLU	2.7
1	A	227	GLY	2.7
1	A	45	PRO	2.7
1	A	136	ASP	2.6
1	B	136	ASP	2.5
1	A	197	ALA	2.5
1	A	369	ASP	2.5
1	A	196	PRO	2.4
1	B	262[A]	LEU	2.4
1	B	216[A]	VAL	2.4
1	A	225	ALA	2.3
1	A	193	PRO	2.3
1	B	230[A]	SER	2.3
1	A	189	GLN	2.2
1	B	201	ASN	2.2
1	A	47	ARG	2.2
1	B	48	VAL	2.1
1	B	172	PRO	2.1
1	A	198	TYR	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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
4	GOL	B	504	6/6	0.84	0.20	22.99	29,42,56,58	0
3	SYN	A	502[B]	8/8	0.86	0.18	8.69	17,22,24,28	8
6	MES	B	505	12/12	0.67	0.21	6.96	40,57,94,99	0
4	GOL	A	503	6/6	0.91	0.16	6.81	23,39,41,42	0
3	SYN	A	502[A]	8/8	0.86	0.18	6.21	17,22,24,28	8
5	PEG	A	505	7/7	0.78	0.22	4.77	35,35,41,42	0
4	GOL	B	501	6/6	0.95	0.12	3.89	19,41,44,61	0
3	SYN	B	503[B]	8/8	0.88	0.19	3.83	21,23,25,30	8
3	SYN	B	503[A]	8/8	0.88	0.19	3.26	21,23,25,30	8
4	GOL	A	506	6/6	0.90	0.10	1.35	22,26,29,33	0
4	GOL	A	504	6/6	0.93	0.12	0.49	19,37,45,51	0
2	HEM	B	502	43/43	0.98	0.08	-0.35	7,9,12,19	0
2	HEM	A	501	43/43	0.98	0.07	-0.41	5,8,12,22	0

## 6.5 Other polymers

There are no such residues in this entry.