



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 PM GMT

PDB ID : 3VLL  
Title : Crystal Structure Analysis of the Ser305Ala variant of KatG from HALOAR-CULA MARISMORTUI Complexes with Inhibitor SHA  
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.  
Deposited on : 2011-12-01  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

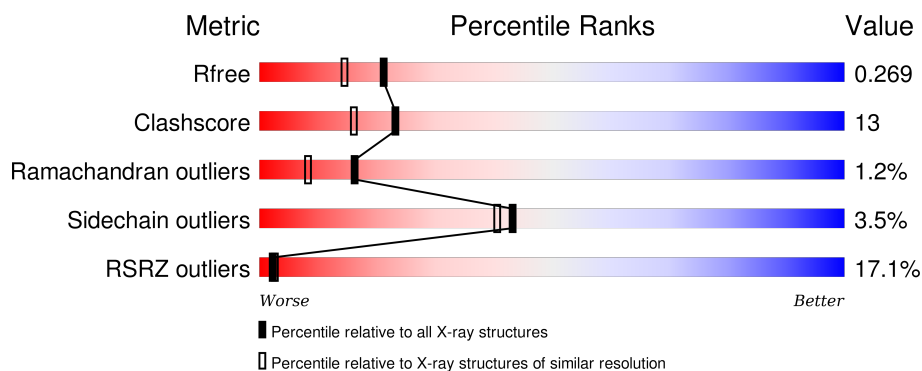
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	737	
1	B	737	

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	SHA	A	801	-	-	-	X
3	SHA	B	801	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11483 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 Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5542	3469	929	1126	18			
1	B	710	Total	C	N	O	S	0	0	0
			5591	3497	941	1134	19			

There are 14 discrepancies between the modelled and reference sequences:

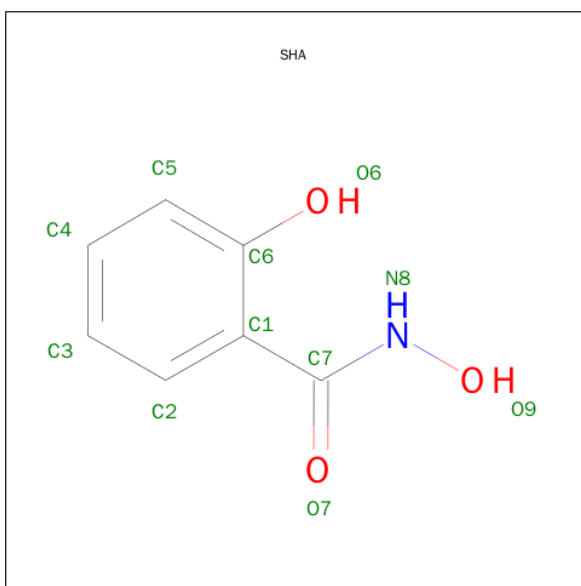
Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	ENGINEERED MUTATION	UNP O59651
A	732	HIS	-	EXPRESSION TAG	UNP O59651
A	733	HIS	-	EXPRESSION TAG	UNP O59651
A	734	HIS	-	EXPRESSION TAG	UNP O59651
A	735	HIS	-	EXPRESSION TAG	UNP O59651
A	736	HIS	-	EXPRESSION TAG	UNP O59651
A	737	HIS	-	EXPRESSION TAG	UNP O59651
B	305	ALA	SER	ENGINEERED MUTATION	UNP O59651
B	732	HIS	-	EXPRESSION TAG	UNP O59651
B	733	HIS	-	EXPRESSION TAG	UNP O59651
B	734	HIS	-	EXPRESSION TAG	UNP O59651
B	735	HIS	-	EXPRESSION TAG	UNP O59651
B	736	HIS	-	EXPRESSION TAG	UNP O59651
B	737	HIS	-	EXPRESSION TAG	UNP O59651

- 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 SALICYLHYDROXAMIC ACID (three-letter code: SHA) (formula:  $C_7H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

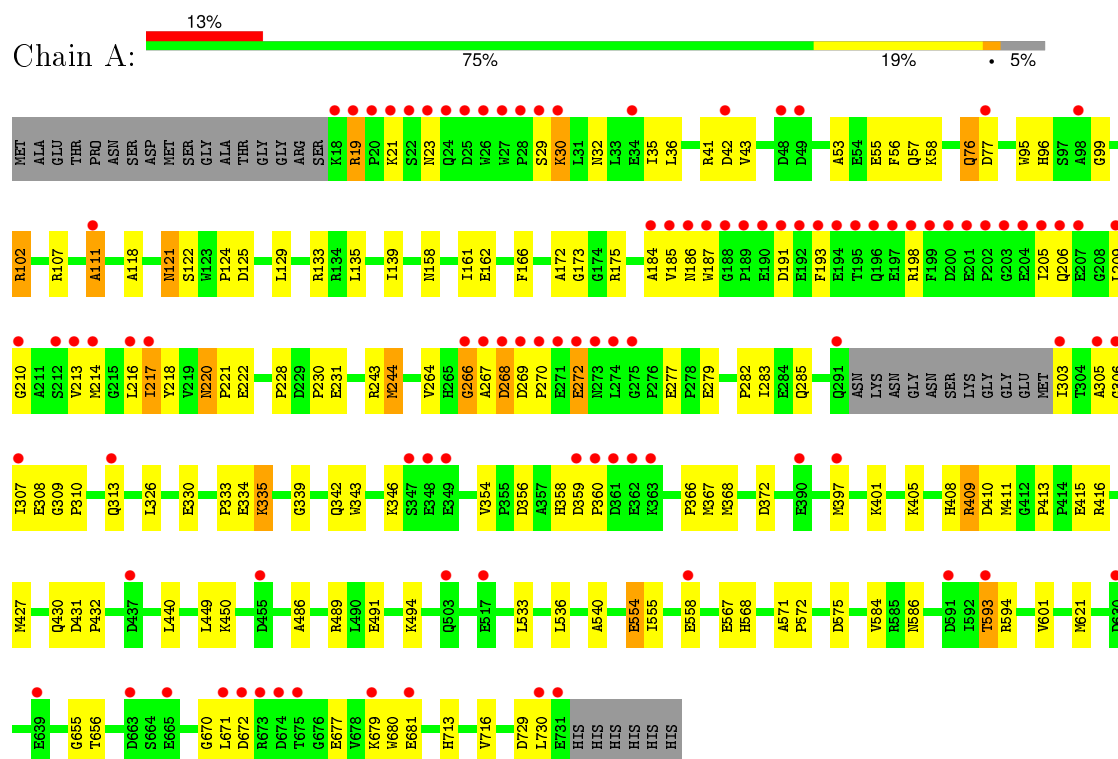
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	93	Total 93	O 93	0	0

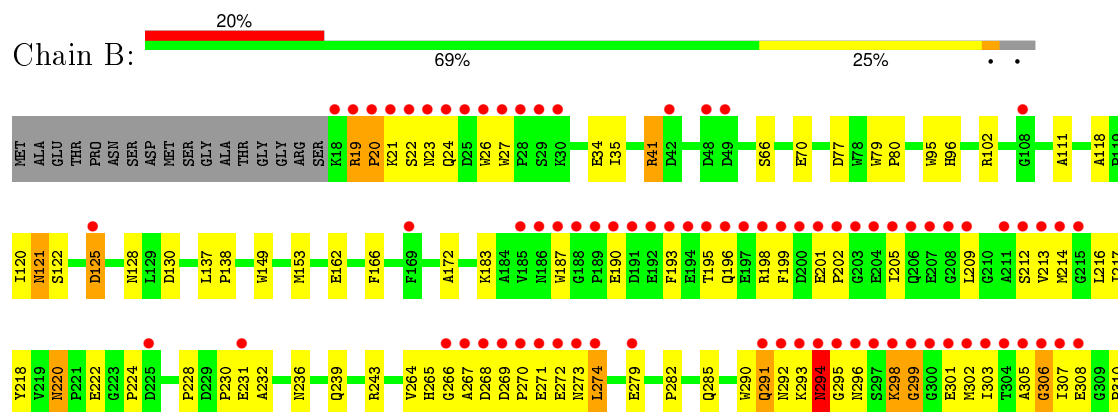
### 3 Residue-property plots

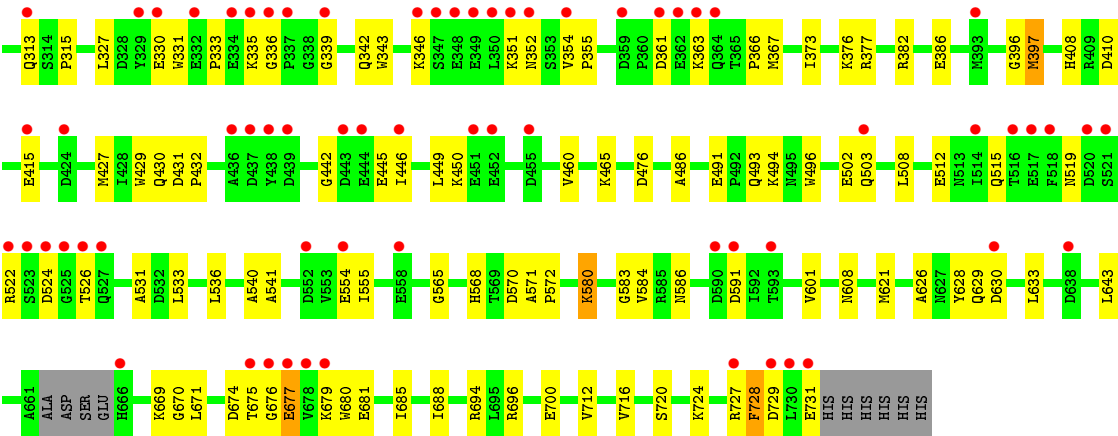
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Catalase-peroxidase 2



#### • Molecule 1: Catalase-peroxidase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.19Å 76.32Å 140.24Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	48.36 – 2.00 48.36 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.36-2.00) 96.2 (48.36-1.79)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247 , 0.271 0.246 , 0.269	Depositor DCC
$R_{free}$ test set	5261 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 45.7	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 143684 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, SHA

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	0.39	1/5677 (0.0%)	0.56	0/7716
1	B	0.31	0/5726	0.52	0/7778
All	All	0.35	1/11403 (0.0%)	0.55	0/15494

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ILE	C-N	10.20	1.57	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5542	0	5191	135	0
1	B	5591	0	5244	165	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	11	0	6	1	0
3	B	11	0	6	1	0
4	A	149	0	0	1	0
4	B	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11483	0	10507	291	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 13.

All (291) 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:95:TRP:CH2	1:A:218:TYR:HE1	1.08	1.66
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.10	1.62
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.01	1.62
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.11	1.60
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.87	1.46
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.96	1.22
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.41	0.98
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.45	0.97
1:A:270:PRO:HG3	1:A:305:ALA:HA	1.48	0.94
1:A:310:PRO:HG3	1:A:354:VAL:HG11	1.51	0.92
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.49	0.92
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.87	0.91
1:A:427:MET:H	1:A:430:GLN:HE21	1.17	0.91
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.52	0.90
1:A:267:ALA:H	1:A:303:ILE:HG12	1.36	0.88
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.91	0.86
1:A:427:MET:H	1:A:430:GLN:NE2	1.74	0.85
1:A:672:ASP:HB2	1:A:679:LYS:HD3	1.56	0.84
1:A:266:GLY:HA2	1:A:303:ILE:HA	1.59	0.83
1:A:172:ALA:H	1:A:408:HIS:HE1	1.27	0.81
1:B:310:PRO:HG3	1:B:354:VAL:HG11	1.61	0.81
1:B:19:ARG:H	1:B:19:ARG:HD3	1.47	0.80
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.68	0.77
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.67	0.77
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.66	0.76
1:B:670:GLY:O	1:B:679:LYS:HB3	1.84	0.76
1:B:270:PRO:HB3	1:B:306:GLY:HA3	1.67	0.76
1:A:43:VAL:HG21	1:B:694:ARG:NH2	2.00	0.76
1:A:326:LEU:HD13	1:A:368:MET:HE2	1.68	0.75
1:B:282:PRO:HD2	1:B:285:GLN:NE2	2.02	0.74
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.72	0.74
1:A:397:MET:HE2	1:A:401:LYS:HG3	1.69	0.74
1:A:217:ILE:HG23	1:A:218:TYR:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:H	1:B:274:LEU:HD12	1.52	0.74
1:A:264:VAL:HG21	1:A:307:ILE:HG22	1.68	0.73
1:B:269:ASP:HB3	1:B:272:GLU:HB2	1.70	0.73
1:A:267:ALA:N	1:A:303:ILE:HG12	2.04	0.72
1:B:679:LYS:HG2	1:B:680:TRP:H	1.54	0.72
1:A:191:ASP:HA	1:B:21:LYS:NZ	2.03	0.72
1:B:266:GLY:HA2	1:B:303:ILE:HG23	1.74	0.70
1:B:565:GLY:H	1:B:568:HIS:HD2	1.39	0.70
1:B:583:GLY:HA2	1:B:685:ILE:HD13	1.73	0.70
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.74	0.69
1:A:269:ASP:HB3	1:A:272:GLU:OE1	1.93	0.69
1:B:265:HIS:HB3	1:B:303:ILE:HA	1.74	0.69
1:B:172:ALA:H	1:B:408:HIS:HE1	1.41	0.69
1:B:273:ASN:HB3	1:B:293:LYS:H	1.58	0.68
1:A:326:LEU:HD13	1:A:368:MET:CE	2.23	0.67
1:A:567:GLU:HG2	1:A:568:HIS:CD2	2.31	0.66
1:B:190:GLU:HG2	1:B:196:GLN:HA	1.77	0.65
1:A:41:ARG:HG2	1:B:41:ARG:HD2	1.79	0.65
1:A:671:LEU:O	1:A:672:ASP:HB3	1.96	0.65
1:B:633:LEU:HD23	1:B:681:GLU:HG3	1.79	0.65
1:A:23:ASN:HD22	1:A:30:LYS:HD3	1.62	0.65
1:B:121:ASN:HD22	1:B:122:SER:N	1.95	0.64
1:B:727:ARG:HB3	1:B:727:ARG:HH21	1.62	0.64
1:A:53:ALA:O	1:A:57:GLN:HG3	1.98	0.64
1:A:335:LYS:HB3	1:A:335:LYS:HZ3	1.63	0.64
1:A:593:THR:HG23	1:A:594:ARG:H	1.61	0.64
1:B:580:LYS:H	1:B:580:LYS:HD3	1.64	0.63
1:B:491:GLU:CD	1:B:494:LYS:HE2	2.18	0.63
1:A:656:THR:HA	1:A:672:ASP:HA	1.80	0.62
1:B:239:GLN:HE21	1:B:243:ARG:HH21	1.47	0.61
1:B:220:ASN:HD22	1:B:222:GLU:H	1.45	0.61
1:A:191:ASP:HA	1:B:21:LYS:HZ3	1.63	0.61
1:B:460:VAL:HG13	1:B:541:ALA:HB1	1.82	0.60
1:A:655:GLY:O	1:A:672:ASP:HA	2.01	0.60
1:A:111:ALA:O	1:A:175:ARG:HB3	2.02	0.60
1:B:727:ARG:NH2	1:B:727:ARG:HB3	2.17	0.60
1:B:580:LYS:H	1:B:580:LYS:CD	2.15	0.60
1:B:580:LYS:HD3	1:B:580:LYS:N	2.16	0.60
1:A:186:ASN:HB2	1:B:20:PRO:HG3	1.83	0.60
1:B:290:TRP:O	1:B:292:ASN:N	2.35	0.59
1:A:205:ILE:HB	1:A:243:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLY:O	1:A:308:GLU:HB2	2.03	0.58
1:B:376:LYS:O	1:B:382:ARG:HD3	2.02	0.58
1:B:294:ASN:O	1:B:302:MET:HA	2.03	0.58
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.84	0.58
1:A:99:GLY:C	1:A:217:ILE:HD11	2.24	0.58
1:A:270:PRO:HD3	1:A:306:GLY:H	1.69	0.58
1:A:368:MET:CE	1:A:372:ASP:HB3	2.34	0.58
1:A:397:MET:CE	1:A:401:LYS:HG3	2.32	0.58
1:B:266:GLY:O	1:B:308:GLU:HB2	2.03	0.58
1:B:196:GLN:HB3	1:B:213:VAL:HG22	1.86	0.58
1:B:327:LEU:HD22	1:B:382:ARG:NH2	2.18	0.57
1:B:503:GLN:HG3	4:B:954:HOH:O	2.03	0.57
1:A:121:ASN:HD22	1:A:122:SER:N	2.01	0.57
1:B:198:ARG:HD2	1:B:212:SER:C	2.25	0.57
1:B:231:GLU:OE1	1:B:377:ARG:HD2	2.05	0.56
1:B:354:VAL:HG21	1:B:366:PRO:HG3	1.86	0.56
1:B:335:LYS:HD2	1:B:339:GLY:HA2	1.86	0.56
1:B:213:VAL:HB	1:B:216:LEU:CD1	2.35	0.56
1:B:111:ALA:HB2	1:B:410:ASP:OD2	2.05	0.56
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.76	0.56
1:B:580:LYS:H	1:B:580:LYS:HZ2	1.53	0.56
1:A:107:ARG:HD3	1:A:185:VAL:HG22	1.87	0.56
1:A:111:ALA:HB2	1:A:410:ASP:OD2	2.06	0.56
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.05	0.56
1:B:149:TRP:O	1:B:153:MET:HG3	2.05	0.56
1:B:450:LYS:HZ2	1:B:536:LEU:HD11	1.71	0.56
1:B:427:MET:HG2	1:B:430:GLN:HE21	1.71	0.55
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.88	0.55
1:B:431:ASP:N	1:B:432:PRO:HD3	2.22	0.54
1:A:567:GLU:HG2	1:A:568:HIS:HD2	1.71	0.54
1:B:230:PRO:HB2	1:B:377:ARG:HG3	1.90	0.54
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.86	0.54
1:B:199:PHE:HB3	1:B:205:ILE:HA	1.90	0.54
1:A:220:ASN:C	1:A:220:ASN:HD22	2.10	0.54
1:B:120:ILE:HD11	1:B:187:TRP:CZ2	2.43	0.54
1:A:270:PRO:HG3	1:A:305:ALA:CA	2.30	0.53
1:A:43:VAL:HG21	1:B:694:ARG:HH22	1.72	0.53
1:B:450:LYS:HB2	1:B:450:LYS:HZ2	1.74	0.53
1:B:273:ASN:O	1:B:292:ASN:HA	2.09	0.53
1:B:427:MET:HG2	1:B:430:GLN:NE2	2.23	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:HG3	1:A:135:LEU:CD2	2.40	0.52
1:A:96:HIS:CE1	1:A:125:ASP:O	2.62	0.52
1:A:217:ILE:CG2	1:A:218:TYR:N	2.69	0.52
1:A:670:GLY:O	1:A:679:LYS:O	2.26	0.52
1:A:405:LYS:O	1:A:409:ARG:HB2	2.09	0.52
1:B:476:ASP:CG	1:B:608:ASN:HD21	2.13	0.52
1:B:307:ILE:N	1:B:307:ILE:HD12	2.25	0.52
1:B:450:LYS:HG3	1:B:540:ALA:HB2	1.92	0.52
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.24	0.52
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.09	0.51
1:B:450:LYS:NZ	1:B:536:LEU:HD11	2.25	0.51
1:A:124:PRO:HG2	1:A:193:PHE:HB3	1.93	0.51
1:B:676:GLY:O	1:B:677:GLU:HB2	2.10	0.51
1:B:333:PRO:HG3	1:B:343:TRP:CZ2	2.46	0.50
1:A:282:PRO:HD2	1:A:285:GLN:NE2	2.25	0.50
1:B:354:VAL:CG2	1:B:366:PRO:HG3	2.41	0.50
1:A:216:LEU:HD22	3:A:801:SHA:O6	2.11	0.50
1:A:268:ASP:O	1:A:306:GLY:HA2	2.12	0.50
1:A:308:GLU:H	1:A:342:GLN:HE22	1.59	0.50
1:B:427:MET:CG	1:B:430:GLN:HE21	2.25	0.50
1:B:118:ALA:HB2	1:B:279:GLU:CD	2.31	0.50
1:B:508:LEU:O	1:B:512:GLU:HG3	2.10	0.50
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.94	0.50
1:A:139:ILE:HG13	4:A:1025:HOH:O	2.12	0.49
1:A:558:GLU:OE1	1:A:730:LEU:HD22	2.12	0.49
1:A:217:ILE:HG23	1:A:218:TYR:H	1.73	0.49
1:B:125:ASP:CG	1:B:216:LEU:HA	2.32	0.49
1:B:696:ARG:O	1:B:700:GLU:HG3	2.12	0.49
1:A:335:LYS:HB3	1:A:335:LYS:NZ	2.27	0.49
1:B:330:GLU:HB3	1:B:346:LYS:HD3	1.93	0.49
1:A:35:ILE:HB	1:A:184:ALA:HB2	1.95	0.49
1:B:162:GLU:HA	1:B:166:PHE:O	2.11	0.49
1:B:291:GLN:O	1:B:293:LYS:HE3	2.13	0.49
1:A:220:ASN:ND2	1:A:222:GLU:H	2.11	0.48
1:A:307:ILE:HA	1:A:342:GLN:NE2	2.29	0.48
1:B:34:GLU:CD	1:B:183:LYS:HE2	2.33	0.48
1:B:230:PRO:CB	1:B:377:ARG:HG3	2.43	0.48
1:A:554:GLU:OE1	1:A:554:GLU:HA	2.13	0.48
1:A:122:SER:HB3	1:A:277:GLU:HG3	1.95	0.48
1:A:102:ARG:HD3	1:A:107:ARG:O	2.14	0.48
1:B:193:PHE:O	1:B:195:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LYS:HG2	1:B:352:ASN:ND2	2.28	0.47
1:B:382:ARG:NH2	1:B:386:GLU:OE1	2.47	0.47
1:B:679:LYS:HG2	1:B:680:TRP:N	2.25	0.47
1:A:264:VAL:HG22	1:A:309:GLY:O	2.15	0.47
1:A:198:ARG:NH1	1:A:209:LEU:HD13	2.30	0.47
1:A:413:PRO:HB2	1:A:415:GLU:OE1	2.14	0.47
1:A:335:LYS:HZ3	1:A:339:GLY:HA2	1.80	0.47
1:A:431:ASP:N	1:A:432:PRO:HD3	2.30	0.47
1:A:220:ASN:HD22	1:A:221:PRO:N	2.12	0.47
1:B:80:PRO:HD2	1:B:296:ASN:O	2.15	0.47
1:A:270:PRO:HB3	1:A:303:ILE:HG22	1.97	0.46
1:A:415:GLU:H	1:A:415:GLU:CD	2.19	0.46
1:A:161:ILE:CG2	1:A:166:PHE:HB3	2.45	0.46
1:A:161:ILE:HG22	1:A:166:PHE:HB3	1.96	0.46
1:A:401:LYS:HE3	1:A:427:MET:CE	2.45	0.46
1:B:271:GLU:HA	1:B:274:LEU:HD13	1.96	0.46
1:B:265:HIS:HB3	1:B:303:ILE:CA	2.45	0.46
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.97	0.46
1:A:32:ASN:ND2	1:A:35:ILE:CG2	2.78	0.46
1:B:676:GLY:O	1:B:677:GLU:CB	2.63	0.46
1:B:486:ALA:HB2	1:B:531:ALA:HB2	1.98	0.46
1:A:56:PHE:CZ	1:A:173:GLY:HA3	2.51	0.46
1:B:224:PRO:HG3	1:B:236:ASN:HD22	1.80	0.46
1:B:522:ARG:HG3	1:B:526:THR:O	2.15	0.46
1:A:41:ARG:HD2	1:A:41:ARG:O	2.16	0.46
1:B:352:ASN:O	1:B:363:LYS:HD2	2.15	0.46
1:A:55:GLU:HA	1:A:58:LYS:HD3	1.96	0.46
1:A:334:GLU:O	1:A:334:GLU:HG3	2.16	0.46
1:A:440:LEU:HD22	1:A:440:LEU:N	2.31	0.46
1:B:22:SER:HB3	1:B:24:GLN:NE2	2.30	0.46
1:B:449:LEU:HD22	1:B:533:LEU:HD21	1.98	0.45
1:A:96:HIS:HE1	1:A:125:ASP:O	1.98	0.45
1:B:720:SER:O	1:B:724:LYS:HG2	2.15	0.45
1:A:198:ARG:HG3	1:A:205:ILE:HG23	1.99	0.45
1:A:214:MET:C	1:A:216:LEU:H	2.20	0.45
1:B:352:ASN:HB3	1:B:363:LYS:HB3	1.96	0.45
1:A:335:LYS:NZ	1:A:339:GLY:HA2	2.31	0.45
1:B:198:ARG:HD2	1:B:212:SER:O	2.17	0.45
1:A:491:GLU:HG2	1:A:494:LYS:HE2	1.98	0.45
1:B:354:VAL:HG13	1:B:355:PRO:HD2	1.97	0.45
1:A:427:MET:N	1:A:430:GLN:HE21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLN:C	1:B:315:PRO:HD3	2.37	0.45
1:A:368:MET:HE3	1:A:372:ASP:HB3	1.98	0.45
1:A:228:PRO:O	1:A:230:PRO:HD3	2.16	0.45
1:A:210:GLY:O	1:A:244:MET:HE3	2.17	0.45
1:B:19:ARG:HD3	1:B:19:ARG:N	2.25	0.44
1:B:307:ILE:HG23	1:B:342:GLN:CD	2.38	0.44
1:B:515:GLN:HG2	1:B:519:ASN:ND2	2.32	0.44
1:B:628:TYR:CE1	1:B:629:GLN:HG3	2.51	0.44
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.03	0.44
1:B:121:ASN:C	1:B:121:ASN:HD22	2.19	0.44
1:B:137:LEU:HB3	1:B:138:PRO:HD3	2.00	0.44
1:A:283:ILE:HD11	1:B:688:ILE:N	2.33	0.44
1:B:209:LEU:O	1:B:243:ARG:HD3	2.18	0.44
1:B:66:SER:O	1:B:70:GLU:HG3	2.18	0.44
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.99	0.44
1:B:267:ALA:H	1:B:303:ILE:CD1	2.30	0.44
1:A:354:VAL:CG2	1:A:366:PRO:HG3	2.48	0.44
1:B:228:PRO:O	1:B:230:PRO:HD3	2.18	0.44
1:B:79:TRP:CE3	1:B:296:ASN:HA	2.53	0.44
1:A:449:LEU:HD22	1:A:533:LEU:HD21	1.99	0.44
1:B:23:ASN:HA	1:B:26:TRP:HD1	1.83	0.44
1:B:728:PHE:HA	1:B:731:GLU:CD	2.39	0.44
1:B:121:ASN:C	1:B:121:ASN:ND2	2.72	0.44
1:A:118:ALA:HB2	1:A:279:GLU:HG3	1.99	0.44
1:B:643:LEU:HD23	1:B:712:VAL:HG13	2.00	0.44
1:B:268:ASP:HB3	1:B:273:ASN:ND2	2.33	0.43
1:B:264:VAL:HG21	1:B:307:ILE:HG22	1.99	0.43
1:A:19:ARG:HD3	1:A:19:ARG:H	1.83	0.43
1:B:196:GLN:CG	1:B:213:VAL:HG22	2.48	0.43
1:B:213:VAL:HB	1:B:216:LEU:HG	2.00	0.43
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.17	0.43
1:A:205:ILE:HG22	1:A:206:GLN:N	2.33	0.43
1:B:669:LYS:HA	1:B:669:LYS:HD3	1.86	0.43
1:B:427:MET:HB3	1:B:429:TRP:CD1	2.54	0.43
1:A:356:ASP:HB3	1:A:359:ASP:O	2.18	0.43
1:B:310:PRO:CG	1:B:354:VAL:HG11	2.39	0.43
1:A:121:ASN:C	1:A:121:ASN:HD22	2.19	0.43
1:A:679:LYS:O	1:A:680:TRP:CB	2.66	0.43
1:A:118:ALA:HB2	1:A:279:GLU:CG	2.49	0.43
1:B:493:GLN:HG2	1:B:496:TRP:CH2	2.54	0.43
1:B:415:GLU:HG2	1:B:729:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:GLY:O	1:B:446:ILE:HG13	2.19	0.43
1:B:427:MET:HB3	1:B:429:TRP:NE1	2.34	0.42
1:A:555:ILE:HG12	1:A:716:VAL:HG13	2.01	0.42
1:A:43:VAL:HG21	1:B:694:ARG:HH21	1.78	0.42
1:B:190:GLU:OE2	1:B:196:GLN:HA	2.20	0.42
1:B:331:TRP:HB3	1:B:343:TRP:HB3	2.00	0.42
1:B:224:PRO:HG3	1:B:236:ASN:ND2	2.34	0.42
1:A:41:ARG:HB3	1:B:41:ARG:HB3	2.01	0.42
1:B:580:LYS:CD	1:B:580:LYS:N	2.80	0.42
1:A:129:LEU:O	1:A:133:ARG:HG3	2.19	0.42
1:B:298:LYS:O	1:B:299:GLY:C	2.57	0.42
1:A:536:LEU:HD23	1:A:536:LEU:O	2.20	0.42
1:B:291:GLN:OE1	1:B:291:GLN:HA	2.19	0.42
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.54	0.42
1:B:198:ARG:CZ	1:B:209:LEU:HD13	2.49	0.42
1:B:445:GLU:OE1	1:B:526:THR:HG21	2.19	0.42
1:B:96:HIS:NE2	3:B:801:SHA:N8	2.68	0.42
1:A:567:GLU:H	1:A:567:GLU:CD	2.23	0.42
1:A:185:VAL:HG11	1:A:187:TRP:CZ2	2.55	0.42
1:B:515:GLN:HG2	1:B:519:ASN:HD21	1.85	0.42
1:A:118:ALA:HB2	1:A:279:GLU:CD	2.39	0.41
1:A:486:ALA:O	1:A:489:ARG:HG2	2.20	0.41
1:B:397:MET:HA	1:B:397:MET:CE	2.50	0.41
1:B:301:GLU:H	1:B:301:GLU:HG2	1.61	0.41
1:A:397:MET:HE2	1:A:397:MET:O	2.19	0.41
1:B:172:ALA:N	1:B:408:HIS:HE1	2.13	0.41
1:B:220:ASN:C	1:B:220:ASN:HD22	2.22	0.41
1:B:352:ASN:HB3	1:B:363:LYS:CB	2.51	0.41
1:A:118:ALA:HA	1:A:121:ASN:ND2	2.35	0.41
1:A:220:ASN:HD22	1:A:222:GLU:H	1.69	0.41
1:A:411:MET:O	1:A:416:ARG:HD3	2.20	0.41
1:B:343:TRP:CD2	1:B:373:ILE:HG13	2.56	0.41
1:B:465:LYS:NZ	1:B:630:ASP:OD2	2.54	0.41
1:B:502:GLU:HG2	1:B:503:GLN:N	2.36	0.41
1:B:196:GLN:HG2	1:B:213:VAL:HG22	2.03	0.41
1:A:231:GLU:H	1:A:231:GLU:CD	2.24	0.41
1:A:333:PRO:HG3	1:A:343:TRP:CH2	2.56	0.41
1:A:330:GLU:HB2	1:A:346:LYS:HD2	2.02	0.41
1:A:358:HIS:O	1:A:360:PRO:HD3	2.21	0.41
1:B:310:PRO:O	1:B:366:PRO:HA	2.21	0.41
1:B:274:LEU:H	1:B:274:LEU:CD1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:C	1:A:121:ASN:ND2	2.74	0.41
1:B:674:ASP:O	1:B:677:GLU:OE1	2.38	0.41
1:B:330:GLU:CB	1:B:346:LYS:HD3	2.50	0.41
1:A:217:ILE:CG2	1:A:218:TYR:H	2.32	0.41
1:A:450:LYS:HG3	1:A:540:ALA:HB2	2.02	0.41
1:A:35:ILE:HG13	1:A:36:LEU:N	2.35	0.40
1:A:158:ASN:O	1:A:162:GLU:HG3	2.22	0.40
1:A:270:PRO:HD3	1:A:306:GLY:N	2.34	0.40
1:A:368:MET:HE1	1:A:372:ASP:HB3	2.04	0.40
1:B:294:ASN:HD22	1:B:294:ASN:HA	1.56	0.40
1:B:621:MET:HG3	1:B:626:ALA:HB3	2.04	0.40
1:B:166:PHE:HZ	1:B:396:GLY:O	2.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	699/737 (95%)	665 (95%)	30 (4%)	4 (1%)	30	22
1	B	706/737 (96%)	650 (92%)	43 (6%)	13 (2%)	11	4
All	All	1405/1474 (95%)	1315 (94%)	73 (5%)	17 (1%)	16	8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	B	305	ALA
1	A	268	ASP
1	B	291	GLN
1	B	591	ASP
1	B	677	GLU

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Mol	Chain	Res	Type
1	A	111	ALA
1	B	294	ASN
1	B	299	GLY
1	B	524	ASP
1	B	274	LEU
1	B	306	GLY
1	A	29	SER
1	B	20	PRO
1	B	336	GLY
1	B	295	GLY
1	A	266	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	581/607 (96%)	559 (96%)	22 (4%)	40	36
1	B	586/607 (96%)	567 (97%)	19 (3%)	46	44
All	All	1167/1214 (96%)	1126 (96%)	41 (4%)	43	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	21	LYS
1	A	30	LYS
1	A	42	ASP
1	A	76	GLN
1	A	77	ASP
1	A	102	ARG
1	A	121	ASN
1	A	220	ASN
1	A	244	MET
1	A	272	GLU
1	A	335	LYS

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Mol	Chain	Res	Type
1	A	367	MET
1	A	409	ARG
1	A	554	GLU
1	A	575	ASP
1	A	586	ASN
1	A	593	THR
1	A	677	GLU
1	A	681	GLU
1	A	713	HIS
1	A	729	ASP
1	B	19	ARG
1	B	41	ARG
1	B	77	ASP
1	B	102	ARG
1	B	121	ASN
1	B	125	ASP
1	B	201	GLU
1	B	214	MET
1	B	220	ASN
1	B	294	ASN
1	B	361	ASP
1	B	367	MET
1	B	397	MET
1	B	554	GLU
1	B	580	LYS
1	B	586	ASN
1	B	671	LEU
1	B	675	THR
1	B	728	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	38	GLN
1	A	57	GLN
1	A	121	ASN
1	A	145	GLN
1	A	220	ASN
1	A	227	ASN
1	A	273	ASN
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	324	ASN
1	A	342	GLN
1	A	352	ASN
1	A	389	GLN
1	A	408	HIS
1	A	430	GLN
1	A	513	ASN
1	A	515	GLN
1	A	527	GLN
1	A	568	HIS
1	A	586	ASN
1	B	24	GLN
1	B	121	ASN
1	B	196	GLN
1	B	220	ASN
1	B	285	GLN
1	B	286	GLN
1	B	313	GLN
1	B	324	ASN
1	B	352	ASN
1	B	358	HIS
1	B	389	GLN
1	B	408	HIS
1	B	430	GLN
1	B	513	ASN
1	B	515	GLN
1	B	568	HIS
1	B	586	ASN
1	B	603	ASN
1	B	608	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	800	1	30,50,50	2.82	10 (33%)	24,82,82	8.03	17 (70%)
3	SHA	A	801	-	11,11,11	1.68	3 (27%)	13,14,14	0.48	0
2	HEM	B	800	1	30,50,50	3.42	11 (36%)	24,82,82	9.63	19 (79%)
3	SHA	B	801	-	11,11,11	1.56	2 (18%)	13,14,14	0.52	0

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	800	1	-	0/10/54/54	0/0/8/8
3	SHA	A	801	-	-	0/6/6/6	0/1/1/1
2	HEM	B	800	1	-	0/10/54/54	0/0/8/8
3	SHA	B	801	-	-	0/6/6/6	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	C3B-C4B	-7.12	1.45	1.51
2	B	800	HEM	C2D-C3D	-6.46	1.35	1.54
2	A	800	HEM	C2D-C3D	-6.25	1.35	1.54
2	A	800	HEM	C3B-C4B	-5.75	1.46	1.51
2	A	800	HEM	C2C-C1C	-4.08	1.44	1.52
2	B	800	HEM	C2C-C1C	-3.85	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C3D-C4D	-3.51	1.47	1.51
2	B	800	HEM	C3D-C4D	-3.51	1.47	1.51
2	B	800	HEM	C2B-C1B	-2.11	1.45	1.51
3	A	801	SHA	C2-C1	2.00	1.43	1.39
3	A	801	SHA	C7-N8	2.79	1.36	1.32
3	B	801	SHA	C7-N8	3.05	1.36	1.32
3	A	801	SHA	C1-C6	3.22	1.46	1.41
3	B	801	SHA	C1-C6	3.25	1.46	1.41
2	B	800	HEM	C1C-NC	3.51	1.40	1.36
2	A	800	HEM	FE-NB	3.65	2.16	1.97
2	A	800	HEM	C1C-NC	3.74	1.40	1.36
2	A	800	HEM	FE-ND	3.87	2.18	1.97
2	B	800	HEM	FE-ND	4.26	2.20	1.97
2	B	800	HEM	CBB-CAB	4.42	1.54	1.29
2	A	800	HEM	CBB-CAB	4.64	1.56	1.29
2	A	800	HEM	CBC-CAC	4.64	1.56	1.29
2	B	800	HEM	CBC-CAC	4.67	1.56	1.29
2	A	800	HEM	FE-NC	5.72	2.18	1.95
2	B	800	HEM	FE-NB	7.70	2.38	1.97
2	B	800	HEM	FE-NC	8.93	2.30	1.95

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	CAA-C2A-C1A	-13.40	112.45	127.01
2	B	800	HEM	CAA-C2A-C1A	-10.18	115.95	127.01
2	B	800	HEM	CHC-C4B-NB	-8.26	104.62	124.52
2	A	800	HEM	CHC-C4B-NB	-7.75	105.85	124.52
2	B	800	HEM	CHD-C1D-ND	-7.02	107.61	124.52
2	A	800	HEM	C3C-CAC-CBC	-6.68	114.21	124.46
2	A	800	HEM	CHD-C1D-ND	-5.68	110.85	124.52
2	A	800	HEM	CAA-CBA-CGA	-5.67	102.35	112.75
2	B	800	HEM	CAA-CBA-CGA	-4.24	104.97	112.75
2	B	800	HEM	C3B-C4B-NB	-4.17	103.64	111.63
2	B	800	HEM	CMA-C3A-C4A	-2.86	123.64	128.36
2	B	800	HEM	C2C-C1C-NC	-2.54	105.93	110.21
2	A	800	HEM	CMA-C3A-C2A	2.37	130.19	125.24
2	A	800	HEM	CBA-CAA-C2A	2.53	117.07	112.53
2	A	800	HEM	CMD-C2D-C3D	2.65	126.08	114.35
2	B	800	HEM	CBA-CAA-C2A	2.84	117.62	112.53
2	B	800	HEM	CMD-C2D-C3D	3.21	128.55	114.35
2	B	800	HEM	CMA-C3A-C2A	4.09	133.78	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C3B-CAB-CBB	4.46	131.29	124.46
2	B	800	HEM	CMC-C2C-C3C	6.52	132.79	116.53
2	B	800	HEM	CAD-C3D-C2D	6.82	132.84	113.22
2	A	800	HEM	CMC-C2C-C3C	6.85	133.63	116.53
2	A	800	HEM	C2D-C3D-C4D	7.38	114.01	101.50
2	A	800	HEM	CAD-C3D-C2D	7.51	134.82	113.22
2	B	800	HEM	C2D-C3D-C4D	7.62	114.42	101.50
2	A	800	HEM	CMB-C2B-C3B	7.90	136.24	116.53
2	B	800	HEM	CMB-C2B-C3B	8.18	136.95	116.53
2	A	800	HEM	C3B-CAB-CBB	8.76	137.90	124.46
2	A	800	HEM	C2C-C1C-CHC	9.13	137.56	123.68
2	A	800	HEM	C3B-C4B-CHC	13.26	141.83	123.16
2	B	800	HEM	C2C-C1C-CHC	15.18	146.78	123.68
2	A	800	HEM	C4B-CHC-C1C	17.22	154.61	125.82
2	A	800	HEM	C1D-CHD-C4C	18.05	155.99	125.82
2	B	800	HEM	C3B-C4B-CHC	20.25	151.66	123.16
2	B	800	HEM	C1D-CHD-C4C	21.07	161.04	125.82
2	B	800	HEM	C4B-CHC-C1C	24.50	166.77	125.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	SHA	1	0
3	B	801	SHA	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	703/737 (95%)	0.85	97 (13%) 4 4	16, 27, 68, 78	0
1	B	710/737 (96%)	1.36	145 (20%) 1 1	17, 35, 72, 80	0
All	All	1413/1474 (95%)	1.10	242 (17%) 2 2	16, 31, 70, 80	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	SER	17.4
1	A	267	ALA	14.1
1	B	300	GLY	13.6
1	A	273	ASN	13.6
1	B	296	ASN	13.5
1	A	26	TRP	13.4
1	B	305	ALA	13.2
1	B	20	PRO	13.2
1	A	272	GLU	12.5
1	B	273	ASN	12.2
1	A	188	GLY	12.2
1	A	19	ARG	11.9
1	B	299	GLY	11.5
1	B	193	PHE	11.2
1	A	25	ASP	11.1
1	B	298	LYS	11.1
1	B	730	LEU	11.1
1	A	305	ALA	10.7
1	B	26	TRP	10.6
1	B	303	ILE	10.3
1	B	195	THR	10.3
1	B	675	THR	10.2
1	A	192	GLU	10.2
1	A	28	PRO	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	PRO	9.9
1	B	189	PRO	9.9
1	A	20	PRO	9.8
1	A	27	TRP	9.6
1	B	269	ASP	9.5
1	B	270	PRO	9.3
1	B	307	ILE	9.0
1	B	295	GLY	8.7
1	B	294	ASN	8.7
1	A	29	SER	8.6
1	A	204	GLU	8.6
1	B	192	GLU	8.6
1	B	191	ASP	8.5
1	A	730	LEU	8.5
1	B	306	GLY	8.4
1	A	361	ASP	8.4
1	A	189	PRO	8.2
1	B	678	VAL	8.2
1	B	292	ASN	8.1
1	B	267	ALA	8.1
1	B	200	ASP	8.0
1	B	268	ASP	8.0
1	B	677	GLU	7.9
1	A	195	THR	7.8
1	B	293	LYS	7.7
1	A	274	LEU	7.7
1	B	272	GLU	7.6
1	B	196	GLN	7.4
1	B	187	TRP	7.4
1	B	266	GLY	7.3
1	B	197	GLU	7.2
1	A	269	ASP	7.1
1	A	199	PHE	7.1
1	A	202	PRO	7.0
1	B	25	ASP	6.7
1	B	337	PRO	6.7
1	B	22	SER	6.7
1	A	191	ASP	6.7
1	A	207	GLU	6.6
1	B	523	SER	6.6
1	A	303	ILE	6.6
1	B	729	ASP	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	TRP	6.6
1	B	214	MET	6.5
1	A	360	PRO	6.5
1	B	590	ASP	6.5
1	B	524	ASP	6.5
1	B	28	PRO	6.5
1	B	676	GLY	6.4
1	B	362	GLU	6.3
1	A	675	THR	6.3
1	A	271	GLU	6.2
1	B	349	GLU	6.2
1	A	203	GLY	6.2
1	B	274	LEU	6.2
1	A	731	GLU	6.2
1	B	301	GLU	6.2
1	A	663	ASP	6.1
1	B	207	GLU	6.1
1	A	674	ASP	6.1
1	A	200	ASP	6.0
1	B	205	ILE	6.0
1	B	731	GLU	5.9
1	B	27	TRP	5.8
1	A	209	LEU	5.8
1	A	291	GLN	5.8
1	B	437	ASP	5.8
1	B	302	MET	5.7
1	B	213	VAL	5.7
1	B	19	ARG	5.6
1	B	188	GLY	5.6
1	B	21	LYS	5.6
1	A	193	PHE	5.5
1	A	213	VAL	5.5
1	B	190	GLU	5.5
1	B	339	GLY	5.3
1	A	205	ILE	5.2
1	B	18	LYS	5.1
1	A	206	GLN	5.1
1	A	266	GLY	5.0
1	A	437	ASP	5.0
1	B	185	VAL	5.0
1	A	194	GLU	4.9
1	B	24	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	23	ASN	4.8
1	A	362	GLU	4.7
1	B	361	ASP	4.7
1	B	208	GLY	4.7
1	B	334	GLU	4.7
1	B	202	PRO	4.6
1	B	42	ASP	4.6
1	A	201	GLU	4.4
1	B	212	SER	4.4
1	B	346	LYS	4.4
1	B	203	GLY	4.3
1	B	521	SER	4.3
1	B	194	GLU	4.3
1	B	424	ASP	4.3
1	B	516	THR	4.2
1	B	209	LEU	4.2
1	A	190	GLU	4.1
1	A	216	LEU	4.1
1	A	348	GLU	4.0
1	B	451	GLU	4.0
1	B	443	ASP	3.9
1	A	23	ASN	3.9
1	A	673	ARG	3.9
1	A	349	GLU	3.9
1	B	201	GLU	3.9
1	B	199	PHE	3.9
1	B	29	SER	3.9
1	A	197	GLU	3.8
1	A	347	SER	3.7
1	B	198	ARG	3.7
1	B	304	THR	3.6
1	B	350	LEU	3.6
1	B	354	VAL	3.6
1	A	198	ARG	3.6
1	A	359	ASP	3.6
1	B	455	ASP	3.6
1	A	22	SER	3.6
1	A	184	ALA	3.5
1	A	212	SER	3.5
1	B	522	ARG	3.5
1	B	638	ASP	3.5
1	B	514	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	593	THR	3.4
1	B	347	SER	3.4
1	B	444	GLU	3.4
1	A	42	ASP	3.4
1	A	672	ASP	3.4
1	B	520	ASP	3.4
1	B	329	TYR	3.3
1	B	271	GLU	3.3
1	B	348	GLU	3.3
1	A	185	VAL	3.3
1	B	215	GLY	3.2
1	A	665	GLU	3.2
1	B	291	GLN	3.2
1	B	48	ASP	3.1
1	A	306	GLY	3.1
1	A	30	LYS	3.1
1	B	593	THR	3.1
1	A	517	GLU	3.0
1	B	630	ASP	3.0
1	B	211	ALA	3.0
1	A	18	LYS	3.0
1	A	217	ILE	3.0
1	B	204	GLU	3.0
1	A	214	MET	3.0
1	A	196	GLN	2.9
1	B	552	ASP	2.9
1	B	525	GLY	2.9
1	B	517	GLU	2.9
1	B	279	GLU	2.9
1	B	206	GLN	2.8
1	A	111	ALA	2.8
1	B	727	ARG	2.8
1	B	30	LYS	2.7
1	B	518	PHE	2.7
1	B	169	PHE	2.7
1	A	186	ASN	2.6
1	B	436	ALA	2.6
1	B	526	THR	2.6
1	B	503	GLN	2.6
1	B	231	GLU	2.6
1	B	679	LYS	2.6
1	A	24	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	351	LYS	2.6
1	A	268	ASP	2.6
1	B	308	GLU	2.5
1	B	364	GLN	2.5
1	B	225	ASP	2.5
1	B	363	LYS	2.5
1	B	186	ASN	2.5
1	B	359	ASP	2.5
1	A	390	GLU	2.5
1	A	77	ASP	2.5
1	A	307	ILE	2.5
1	B	313	GLN	2.5
1	B	591	ASP	2.4
1	A	98	ALA	2.4
1	A	503	GLN	2.4
1	B	49	ASP	2.4
1	B	332	GLU	2.4
1	A	275	GLY	2.4
1	B	438	TYR	2.4
1	B	415	GLU	2.4
1	B	335	LYS	2.3
1	A	363	LYS	2.3
1	B	527	GLN	2.3
1	A	630	ASP	2.2
1	B	352	ASN	2.2
1	A	34	GLU	2.2
1	B	439	ASP	2.2
1	A	558	GLU	2.2
1	A	681	GLU	2.2
1	A	210	GLY	2.2
1	A	455	ASP	2.2
1	A	49	ASP	2.2
1	A	591	ASP	2.1
1	A	397	MET	2.1
1	A	679	LYS	2.1
1	B	330	GLU	2.1
1	B	452	GLU	2.1
1	A	639	GLU	2.1
1	B	125	ASP	2.1
1	B	666	HIS	2.1
1	A	21	LYS	2.1
1	B	336	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLN	2.1
1	B	558	GLU	2.0
1	A	671	LEU	2.0
1	B	393	MET	2.0
1	B	554	GLU	2.0
1	B	108	GLY	2.0
1	A	48	ASP	2.0
1	B	446	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SHA	B	801	11/11	0.67	0.25	2.00	49,51,51,51	11
3	SHA	A	801	11/11	0.47	0.53	1.72	52,52,52,53	11
2	HEM	A	800	43/43	0.96	0.15	0.40	15,21,30,39	0
2	HEM	B	800	43/43	0.96	0.12	-0.22	21,29,36,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.