



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:40 AM GMT

PDB ID : 3MQE  
Title : Structure of SC-75416 bound at the COX-2 active site  
Authors : Wang, J.L.; Limburg, D.; Graneto, M.J.; Springer, J.; Rogier, J.; Kiefer, J.R.  
Deposited on : 2010-04-28  
Resolution : 2.80 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

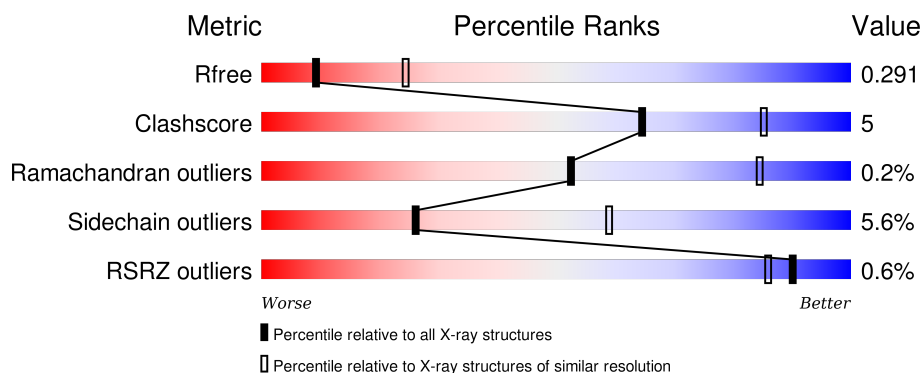
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	587	<div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	B	587	<div> <div>80%</div> <div>12%</div> <div>6%</div> </div>
1	C	587	<div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
1	D	587	<div> <div>81%</div> <div>11%</div> <div>6%</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	NAG	A	661	X	-	-	-
3	NAG	A	681	-	-	-	X
3	NAG	B	661	X	-	-	-
3	NAG	B	681	-	-	-	X
3	NAG	C	661	X	-	-	X
3	NAG	D	661	X	-	-	-
3	NAG	D	681	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18573 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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



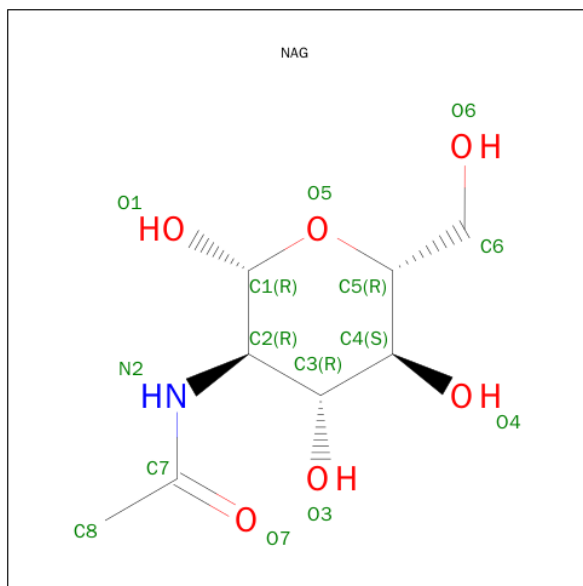
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

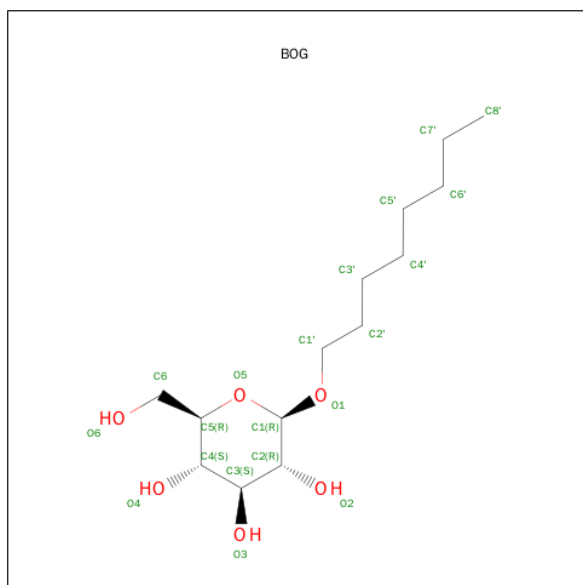


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

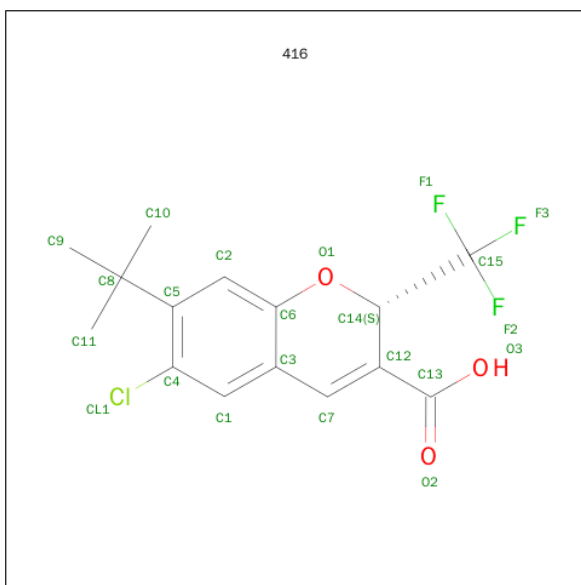
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			42	24	3	15		
4	B	3	Total	C	N	O	0	0
			42	24	3	15		
4	C	3	Total	C	N	O	0	0
			42	24	3	15		
4	D	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is (2S)-7-TERT-BUTYL-6-CHLORO-2-(TRIFLUOROMETHYL)-2H-CHROMENE-3-CARBOXYLIC ACID (three-letter code: 416) (formula:  $C_{15}H_{14}ClF_3O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	F	O	0	0
			22	15	1	3	3		
6	B	1	Total	C	Cl	F	O	0	0
			22	15	1	3	3		
6	C	1	Total	C	Cl	F	O	0	0
			22	15	1	3	3		
6	D	1	Total	C	Cl	F	O	0	0
			22	15	1	3	3		

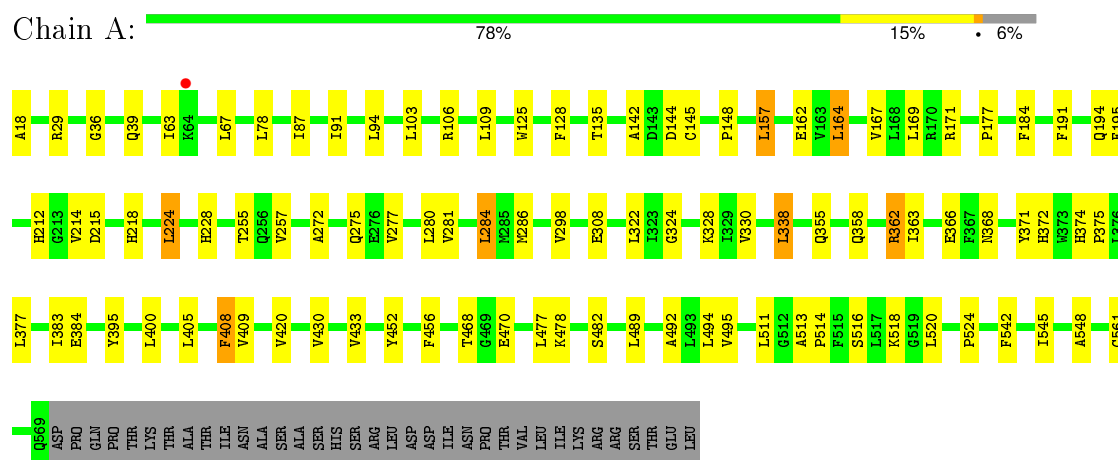
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total	O	0	0
			31	31		
7	B	24	Total	O	0	0
			24	24		
7	C	23	Total	O	0	0
			23	23		
7	D	19	Total	O	0	0
			19	19		

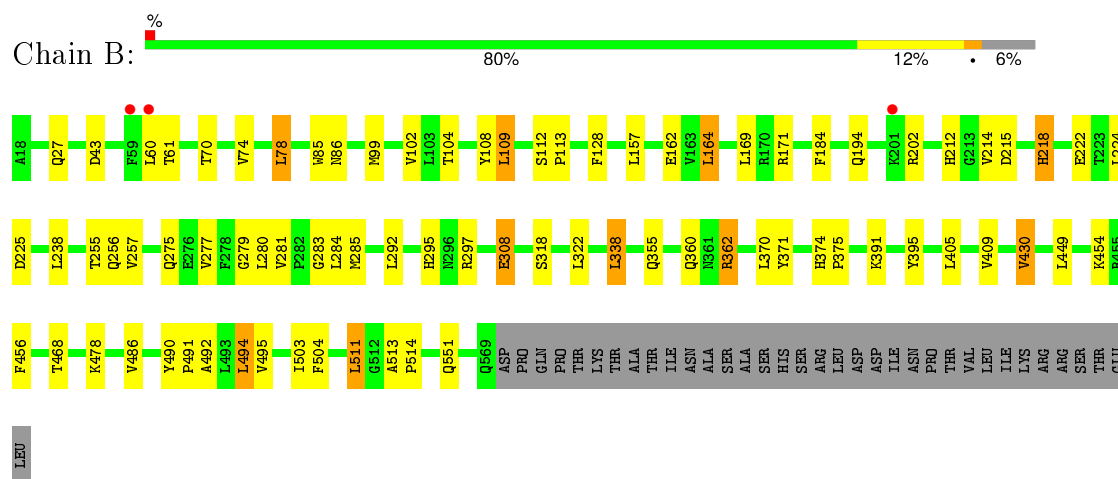
### 3 Residue-property plots

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.

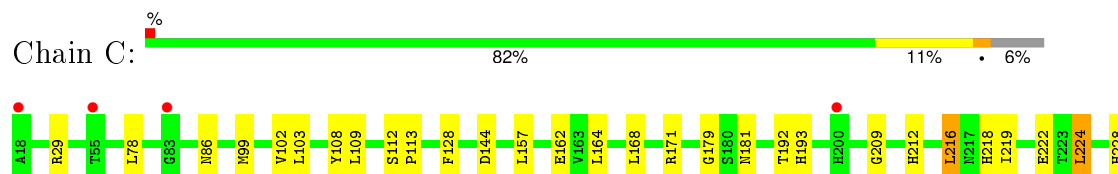
#### • Molecule 1: Prostaglandin G/H synthase 2



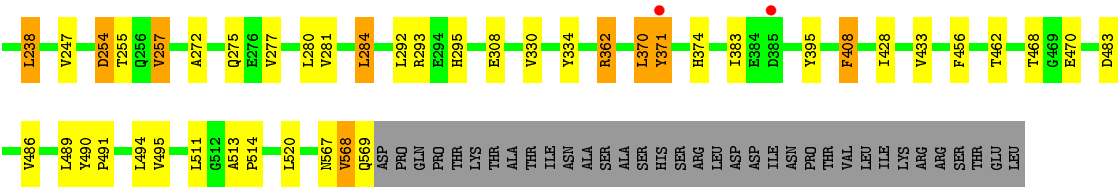
#### • Molecule 1: Prostaglandin G/H synthase 2



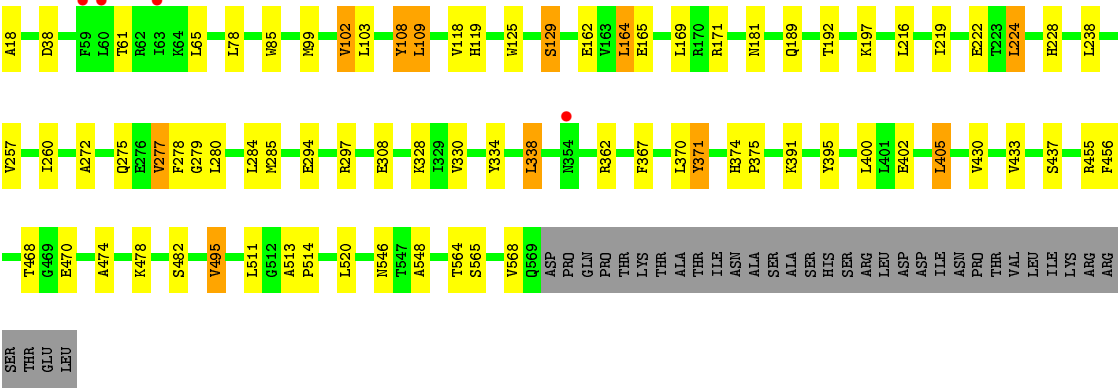
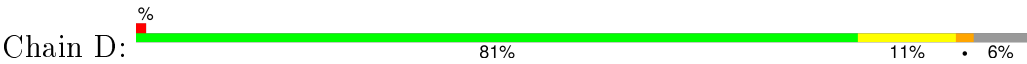
#### • Molecule 1: Prostaglandin G/H synthase 2







• Molecule 1: Prostaglandin G/H synthase 2



SER  
THR  
GLU  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.70Å 140.38Å 129.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 34.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.80) 99.1 (34.28-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.236 , 0.290 0.234 , 0.291	Depositor DCC
$R_{free}$ test set	8264 reflections (11.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 82407 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8586e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 416, NAG, BOG

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	0.50	0/4601	0.62	1/6239 (0.0%)
1	B	0.50	0/4601	0.60	0/6239
1	C	0.47	0/4601	0.58	0/6239
1	D	0.48	0/4601	0.59	0/6239
All	All	0.49	0/18404	0.60	1/24956 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASP	CB-CG-OD1	5.34	123.11	118.30

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	4474	0	4373	50	0
1	B	4474	0	4373	46	0
1	C	4474	0	4373	42	0
1	D	4474	0	4373	40	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	1	0
2	D	43	0	30	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	42	0	37	0	0
4	B	42	0	37	0	0
4	C	42	0	37	0	0
4	D	42	0	37	1	0
5	A	20	0	28	0	0
5	C	20	0	28	0	0
6	A	22	0	13	2	0
6	B	22	0	13	2	0
6	C	22	0	13	1	0
6	D	22	0	13	3	0
7	A	31	0	0	0	0
7	B	24	0	0	1	0
7	C	23	0	0	0	0
7	D	19	0	0	0	0
All	All	18573	0	17972	185	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 5.

All (185) 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:D:328:LYS:NZ	1:D:546:ASN:O	2.13	0.81
1:C:513:ALA:HB3	1:C:514:PRO:HD3	1.63	0.80
1:B:128:PHE:O	1:B:362:ARG:NH2	2.18	0.76
1:C:179:GLY:O	1:C:568:VAL:HG23	1.85	0.76
1:A:184:PHE:CZ	1:A:338:LEU:HD11	2.22	0.75
1:C:468:THR:HG22	1:C:495:VAL:HG12	1.66	0.74
1:D:257:VAL:CG2	1:D:272:ALA:HB1	2.18	0.74
1:D:257:VAL:HG21	1:D:272:ALA:HB1	1.74	0.70
1:A:468:THR:HG22	1:A:495:VAL:CG1	2.23	0.68
1:A:164:LEU:HD22	1:A:169:LEU:HG	1.75	0.67
1:B:27:GLN:HE22	1:B:454:LYS:NZ	1.91	0.67
1:C:255:THR:OG1	1:C:257:VAL:HG12	1.96	0.66
6:B:701:416:CL1	6:B:701:416:H11B	2.32	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD21	2:A:605:HEM:HBB2	1.78	0.66
1:A:456:PHE:CG	1:A:511:LEU:HD22	2.31	0.66
1:D:109:LEU:O	1:D:455:ARG:NH2	2.29	0.65
1:D:197:LYS:HZ1	1:D:222:GLU:HG3	1.62	0.64
1:A:191:PHE:O	1:A:194:GLN:NE2	2.30	0.63
1:C:277:VAL:HG23	1:C:280:LEU:HD12	1.81	0.63
1:C:483:ASP:HB3	1:C:486:VAL:HG23	1.81	0.62
1:C:128:PHE:O	1:C:362:ARG:NH2	2.32	0.62
1:D:189:GLN:CD	1:D:284:LEU:HD11	2.21	0.61
1:B:275:GLN:OE1	1:B:277:VAL:HG12	2.01	0.61
1:A:328:LYS:HG2	1:A:548:ALA:HB3	1.82	0.61
1:B:184:PHE:CZ	1:B:338:LEU:HD11	2.36	0.60
1:C:192:THR:HG21	1:C:371:TYR:CE2	2.37	0.60
1:A:128:PHE:O	1:A:362:ARG:NH2	2.34	0.60
1:D:468:THR:HG22	1:D:495:VAL:HG13	1.84	0.59
1:B:456:PHE:CG	1:B:511:LEU:HD22	2.37	0.59
1:A:330:VAL:HG11	1:A:520:LEU:HD11	1.85	0.59
1:B:238:LEU:HD13	1:B:295:HIS:CD2	2.38	0.59
1:D:328:LYS:HG2	1:D:548:ALA:HB3	1.86	0.58
1:B:491:PRO:O	1:B:495:VAL:HG23	2.03	0.58
1:A:87:ILE:HG22	1:A:91:ILE:HD12	1.86	0.57
1:C:456:PHE:CG	1:C:511:LEU:HD22	2.40	0.57
1:C:257:VAL:CG1	1:C:272:ALA:HB1	2.35	0.56
1:C:257:VAL:HG11	1:C:272:ALA:HB1	1.87	0.56
6:C:701:416:CL1	6:C:701:416:H11B	2.42	0.56
1:D:260:ILE:HD12	1:D:277:VAL:HG23	1.88	0.56
1:C:280:LEU:HD22	1:C:395:TYR:CE2	2.41	0.56
1:B:281:VAL:HG12	1:B:283:GLY:H	1.70	0.56
1:A:286:MET:HE1	1:A:409:VAL:HG22	1.88	0.56
1:D:456:PHE:CD2	1:D:511:LEU:HD22	2.41	0.56
1:C:216:LEU:CD1	1:C:219:ILE:HD12	2.35	0.55
1:D:279:GLY:HA2	1:D:285:MET:CE	2.36	0.55
6:A:701:416:CL1	6:A:701:416:H11B	2.43	0.55
1:C:181:ASN:HB3	1:C:568:VAL:HG22	1.87	0.55
1:A:224:LEU:HD22	1:A:228:HIS:CD2	2.41	0.55
1:C:383:ILE:HD13	1:C:408:PHE:CE1	2.42	0.55
1:D:513:ALA:HB3	1:D:514:PRO:HD3	1.88	0.55
1:B:164:LEU:HD22	1:B:169:LEU:HG	1.90	0.54
1:D:374:HIS:CE1	1:D:433:VAL:HG11	2.41	0.54
1:C:112:SER:HA	1:C:113:PRO:C	2.28	0.54
1:D:400:LEU:HD11	1:D:405:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:THR:HG22	1:B:495:VAL:HG12	1.90	0.53
1:A:377:LEU:CD2	2:A:605:HEM:HBB2	2.39	0.53
1:B:318:SER:O	1:B:322:LEU:HD13	2.08	0.53
1:B:255:THR:O	1:B:256:GLN:HB2	2.07	0.53
1:C:456:PHE:CD2	1:C:511:LEU:HD22	2.43	0.53
1:D:192:THR:HG21	1:D:371:TYR:CE2	2.44	0.53
1:C:374:HIS:CE1	1:C:433:VAL:HG11	2.44	0.52
1:A:125:TRP:CZ2	1:B:215:ASP:HB3	2.45	0.52
1:A:257:VAL:HG21	1:A:272:ALA:HB1	1.91	0.52
2:C:605:HEM:HBC2	2:C:605:HEM:HHD	1.91	0.52
1:A:358:GLN:O	1:A:518:LYS:NZ	2.42	0.51
1:B:225:ASP:HB2	7:B:612:HOH:O	2.09	0.51
1:B:99:MET:O	1:B:102:VAL:HG22	2.10	0.51
1:D:280:LEU:HD22	1:D:395:TYR:CE2	2.46	0.51
1:D:338:LEU:HD23	6:D:701:416:H14	1.93	0.51
1:B:214:VAL:HG12	1:B:214:VAL:O	2.10	0.51
1:C:277:VAL:CG2	1:C:280:LEU:HD12	2.41	0.51
1:B:280:LEU:HD22	1:B:395:TYR:CD2	2.46	0.51
1:C:280:LEU:HD22	1:C:395:TYR:HE2	1.76	0.50
1:A:214:VAL:O	1:A:214:VAL:HG12	2.12	0.50
1:C:108:TYR:CE2	1:C:109:LEU:HD22	2.46	0.50
1:C:468:THR:HG22	1:C:495:VAL:CG1	2.38	0.50
1:B:374:HIS:N	1:B:375:PRO:CD	2.73	0.50
1:B:99:MET:HE3	1:B:102:VAL:HG21	1.94	0.50
1:D:456:PHE:CG	1:D:511:LEU:HD22	2.46	0.50
1:A:374:HIS:N	1:A:375:PRO:CD	2.75	0.50
1:D:18:ALA:HB1	1:D:38:ASP:OD1	2.12	0.49
1:B:375:PRO:HG2	1:B:494:LEU:HD13	1.93	0.49
1:A:280:LEU:HD22	1:A:395:TYR:CE2	2.46	0.49
1:C:224:LEU:HD22	1:C:228:HIS:NE2	2.27	0.49
1:C:216:LEU:HD12	1:C:219:ILE:HD12	1.93	0.49
1:A:36:GLY:C	1:B:308:GLU:HG2	2.33	0.49
1:B:405:LEU:O	1:B:409:VAL:HG23	2.12	0.49
1:D:164:LEU:HD22	1:D:169:LEU:HG	1.94	0.49
1:B:511:LEU:N	1:B:511:LEU:HD23	2.27	0.49
1:B:78:LEU:CD1	1:B:85:TRP:CZ2	2.95	0.49
1:C:292:LEU:C	1:C:292:LEU:HD23	2.33	0.48
1:B:513:ALA:HB3	1:B:514:PRO:HD3	1.95	0.48
1:C:370:LEU:HD12	1:C:370:LEU:C	2.34	0.48
1:A:148:PRO:HG2	1:A:157:LEU:HD22	1.95	0.48
1:D:224:LEU:HD22	1:D:228:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:HA2	1:B:285:MET:CE	2.44	0.48
1:A:516:SER:O	1:A:520:LEU:HD22	2.13	0.48
1:D:374:HIS:N	1:D:375:PRO:CD	2.76	0.48
2:B:605:HEM:HBB2	2:B:605:HEM:CMB	2.44	0.48
1:B:108:TYR:CZ	1:B:109:LEU:HD22	2.49	0.48
1:A:383:ILE:HD13	1:A:408:PHE:CE1	2.49	0.47
1:A:298:VAL:HG21	1:A:322:LEU:HD11	1.96	0.47
1:D:118:VAL:HG13	1:D:119:HIS:CD2	2.50	0.47
1:B:370:LEU:HD12	1:B:370:LEU:C	2.34	0.47
1:D:278:PHE:CD1	1:D:284:LEU:HD23	2.49	0.47
1:D:216:LEU:HB3	1:D:219:ILE:HD12	1.97	0.47
1:A:184:PHE:CE1	1:A:338:LEU:HD11	2.49	0.47
1:D:125:TRP:O	1:D:129:SER:OG	2.32	0.47
1:A:255:THR:HB	1:A:257:VAL:HG13	1.97	0.47
1:A:18:ALA:HB3	1:A:144:ASP:OD2	2.16	0.47
1:C:254:ASP:OD2	1:C:254:ASP:C	2.54	0.46
4:D:672:NAG:H4	4:D:673:NAG:N2	2.30	0.46
1:D:278:PHE:HD1	1:D:284:LEU:HD23	1.80	0.46
1:D:468:THR:OG1	1:D:474:ALA:HB2	2.16	0.46
1:C:212:HIS:CE1	1:C:362:ARG:HD2	2.51	0.46
1:A:524:PRO:HG3	1:B:128:PHE:CE2	2.51	0.46
6:D:701:416:CL1	6:D:701:416:H11B	2.53	0.45
1:B:194:GLN:HB3	1:B:218:HIS:CD2	2.50	0.45
1:A:366:GLU:HG2	1:A:452:TYR:CE1	2.51	0.45
1:A:324:GLY:HA3	1:A:545:ILE:HD13	1.98	0.45
1:A:456:PHE:CD2	1:A:511:LEU:HD22	2.51	0.45
1:B:70:THR:O	1:B:74:VAL:HG23	2.16	0.45
1:A:281:VAL:HB	1:A:284:LEU:HD22	1.98	0.45
1:A:374:HIS:CE1	1:A:433:VAL:HG11	2.52	0.45
1:D:181:ASN:HB3	1:D:568:VAL:HG23	1.98	0.44
1:C:99:MET:O	1:C:102:VAL:HG22	2.17	0.44
1:A:91:ILE:HB	1:A:94:LEU:HD12	2.00	0.44
1:D:165:GLU:HA	1:D:169:LEU:HD12	2.00	0.44
6:D:701:416:H9A	6:D:701:416:CL1	2.55	0.44
1:B:449:LEU:HD22	1:B:492:ALA:CB	2.48	0.44
1:B:456:PHE:CD2	1:B:511:LEU:HD22	2.52	0.44
1:B:112:SER:HA	1:B:113:PRO:C	2.38	0.44
1:C:330:VAL:CG1	1:C:520:LEU:HD21	2.47	0.44
1:B:27:GLN:HE22	1:B:454:LYS:HZ2	1.64	0.44
1:A:513:ALA:HB3	1:A:514:PRO:HD3	1.99	0.44
1:C:490:TYR:HB3	1:C:491:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:HE3	1:B:102:VAL:CG2	2.47	0.43
1:C:209:GLY:HA2	1:C:222:GLU:OE2	2.18	0.43
1:A:368:ASN:O	1:A:372:HIS:HD2	2.01	0.43
1:A:142:ALA:HB3	1:A:145:CYS:SG	2.58	0.43
1:C:238:LEU:HD13	1:C:295:HIS:CD2	2.53	0.43
1:A:257:VAL:CG2	1:A:272:ALA:HB1	2.48	0.43
1:C:281:VAL:HB	1:C:284:LEU:HD22	2.00	0.43
1:D:78:LEU:HD13	1:D:85:TRP:CZ2	2.54	0.43
1:B:430:VAL:HG13	1:B:430:VAL:O	2.19	0.42
1:A:400:LEU:HD11	1:A:405:LEU:HD22	2.00	0.42
1:A:167:VAL:HG21	1:A:477:LEU:HD21	2.00	0.42
1:D:108:TYR:CE2	1:D:109:LEU:HD22	2.55	0.42
1:C:490:TYR:HB3	1:C:491:PRO:HD3	2.01	0.42
1:D:294:GLU:OE1	1:D:297:ARG:NH1	2.52	0.42
1:B:486:VAL:HG12	1:B:486:VAL:O	2.19	0.42
1:A:430:VAL:O	1:A:430:VAL:HG13	2.18	0.42
1:D:99:MET:HE3	1:D:102:VAL:CG2	2.49	0.42
1:B:43:ASP:OD1	1:B:43:ASP:C	2.58	0.42
1:C:330:VAL:O	1:C:334:TYR:HB3	2.20	0.42
1:A:561:CYS:O	1:A:561:CYS:SG	2.78	0.42
1:A:135:THR:HG22	1:A:363:ILE:O	2.20	0.42
1:A:468:THR:HG22	1:A:495:VAL:HG13	2.00	0.42
1:B:490:TYR:N	1:B:491:PRO:HD2	2.34	0.42
1:A:368:ASN:O	1:A:372:HIS:CD2	2.73	0.42
1:D:330:VAL:HA	1:D:334:TYR:HB3	2.01	0.41
1:B:78:LEU:HD12	1:B:85:TRP:CZ2	2.55	0.41
1:B:104:THR:HG22	1:B:355:GLN:HG2	2.02	0.41
1:D:61:THR:O	1:D:65:LEU:HG	2.20	0.41
1:D:257:VAL:HG22	1:D:272:ALA:HB1	1.99	0.41
6:B:701:416:CL1	6:B:701:416:H9A	2.57	0.41
1:D:430:VAL:O	1:D:430:VAL:HG13	2.20	0.41
1:C:568:VAL:O	1:C:568:VAL:HG12	2.21	0.41
1:B:27:GLN:HE22	1:B:454:LYS:HZ1	1.66	0.41
1:A:224:LEU:HD22	1:A:228:HIS:NE2	2.36	0.41
1:B:503:ILE:HG23	1:B:504:PHE:CD2	2.55	0.41
1:C:247:VAL:O	1:C:293:ARG:NH1	2.54	0.41
1:C:489:LEU:O	1:C:489:LEU:HD12	2.21	0.41
1:D:495:VAL:HG13	1:D:495:VAL:O	2.21	0.40
1:A:375:PRO:HB2	1:A:420:VAL:HA	2.03	0.40
1:B:503:ILE:HG23	1:B:504:PHE:CG	2.56	0.40
1:C:374:HIS:CE1	1:C:433:VAL:CG1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HD22	1:C:494:LEU:HD12	2.04	0.40
1:A:63:ILE:O	1:A:67:LEU:HD13	2.21	0.40
1:D:328:LYS:NZ	1:D:546:ASN:C	2.74	0.40
6:A:701:416:CL1	6:A:701:416:H9A	2.58	0.40
1:B:292:LEU:HD23	1:B:292:LEU:C	2.42	0.40
1:C:216:LEU:HD13	1:C:219:ILE:HD12	2.03	0.40
1:A:375:PRO:HG2	1:A:494:LEU:HD22	2.03	0.40
1:A:489:LEU:O	1:A:492:ALA:HB3	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	A	550/587 (94%)	519 (94%)	29 (5%)	2 (0%)	39	74
1	B	550/587 (94%)	519 (94%)	30 (6%)	1 (0%)	52	84
1	C	550/587 (94%)	528 (96%)	21 (4%)	1 (0%)	52	84
1	D	550/587 (94%)	512 (93%)	38 (7%)	0	100	100
All	All	2200/2348 (94%)	2078 (94%)	118 (5%)	4 (0%)	52	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	B	212	HIS
1	A	384	GLU
1	C	568	VAL

### 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	493/525 (94%)	466 (94%)	27 (6%)	27	59
1	B	493/525 (94%)	466 (94%)	27 (6%)	27	59
1	C	493/525 (94%)	465 (94%)	28 (6%)	25	58
1	D	493/525 (94%)	464 (94%)	29 (6%)	24	57
All	All	1972/2100 (94%)	1861 (94%)	111 (6%)	26	59

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	39	GLN
1	A	78	LEU
1	A	103	LEU
1	A	106	ARG
1	A	109	LEU
1	A	157	LEU
1	A	162	GLU
1	A	164	LEU
1	A	171	ARG
1	A	177	PRO
1	A	195	PHE
1	A	218	HIS
1	A	224	LEU
1	A	275	GLN
1	A	277	VAL
1	A	284	LEU
1	A	308	GLU
1	A	338	LEU
1	A	355	GLN
1	A	362	ARG
1	A	371	TYR
1	A	408	PHE
1	A	470	GLU

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Mol	Chain	Res	Type
1	A	478	LYS
1	A	482	SER
1	A	542	PHE
1	B	60	LEU
1	B	61	THR
1	B	78	LEU
1	B	86	ASN
1	B	109	LEU
1	B	157	LEU
1	B	162	GLU
1	B	164	LEU
1	B	171	ARG
1	B	202	ARG
1	B	218	HIS
1	B	222	GLU
1	B	224	LEU
1	B	257	VAL
1	B	284	LEU
1	B	297	ARG
1	B	308	GLU
1	B	338	LEU
1	B	360	GLN
1	B	362	ARG
1	B	371	TYR
1	B	391	LYS
1	B	430	VAL
1	B	478	LYS
1	B	494	LEU
1	B	511	LEU
1	B	551	GLN
1	C	29	ARG
1	C	78	LEU
1	C	86	ASN
1	C	103	LEU
1	C	144	ASP
1	C	157	LEU
1	C	162	GLU
1	C	164	LEU
1	C	171	ARG
1	C	193	HIS
1	C	216	LEU
1	C	218	HIS

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Mol	Chain	Res	Type
1	C	224	LEU
1	C	238	LEU
1	C	254	ASP
1	C	257	VAL
1	C	275	GLN
1	C	284	LEU
1	C	308	GLU
1	C	362	ARG
1	C	370	LEU
1	C	371	TYR
1	C	408	PHE
1	C	428	ILE
1	C	462	THR
1	C	470	GLU
1	C	567	ASN
1	C	569	GLN
1	D	102	VAL
1	D	103	LEU
1	D	108	TYR
1	D	109	LEU
1	D	129	SER
1	D	162	GLU
1	D	164	LEU
1	D	171	ARG
1	D	224	LEU
1	D	238	LEU
1	D	275	GLN
1	D	277	VAL
1	D	308	GLU
1	D	338	LEU
1	D	362	ARG
1	D	367	PHE
1	D	370	LEU
1	D	371	TYR
1	D	391	LYS
1	D	402	GLU
1	D	405	LEU
1	D	437	SER
1	D	470	GLU
1	D	478	LYS
1	D	482	SER
1	D	495	VAL

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Mol	Chain	Res	Type
1	D	520	LEU
1	D	564	THR
1	D	565	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	551	GLN
1	A	569	GLN
1	B	27	GLN
1	B	72	ASN
1	B	264	HIS
1	B	313	GLN
1	B	360	GLN
1	B	374	HIS
1	B	556	ASN
1	B	567	ASN
1	C	190	HIS
1	C	374	HIS
1	C	551	GLN
1	C	569	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 ⓘ

12 carbohydrates 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	$\# Z  > 2$
4	NAG	A	671	1,4	14,14,15	0.46	0	15,19,21	2.62	3 (20%)
4	NAG	A	672	4	14,14,15	0.58	0	15,19,21	1.82	5 (33%)
4	NAG	A	673	4	14,14,15	0.72	1 (7%)	15,19,21	2.02	3 (20%)
4	NAG	B	671	1,4	14,14,15	0.70	0	15,19,21	0.98	0
4	NAG	B	672	4	14,14,15	0.45	0	15,19,21	1.50	2 (13%)
4	NAG	B	673	4	14,14,15	0.91	1 (7%)	15,19,21	1.92	2 (13%)
4	NAG	C	671	1,4	14,14,15	0.64	0	15,19,21	1.73	1 (6%)
4	NAG	C	672	4	14,14,15	0.43	0	15,19,21	1.50	3 (20%)
4	NAG	C	673	4	14,14,15	0.97	2 (14%)	15,19,21	2.52	6 (40%)
4	NAG	D	671	1,4	14,14,15	0.61	0	15,19,21	1.49	2 (13%)
4	NAG	D	672	4	14,14,15	0.67	0	15,19,21	1.52	2 (13%)
4	NAG	D	673	4	14,14,15	0.90	1 (7%)	15,19,21	2.46	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	672	4	-	0/6/23/26	0/1/1/1
4	NAG	A	673	4	-	0/6/23/26	0/1/1/1
4	NAG	B	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	672	4	-	0/6/23/26	0/1/1/1
4	NAG	B	673	4	-	0/6/23/26	0/1/1/1
4	NAG	C	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	672	4	-	0/6/23/26	0/1/1/1
4	NAG	C	673	4	-	0/6/23/26	0/1/1/1
4	NAG	D	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	672	4	-	0/6/23/26	0/1/1/1
4	NAG	D	673	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	673	NAG	C2-N2	2.09	1.50	1.46
4	A	673	NAG	C1-C2	2.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	673	NAG	C1-C2	2.40	1.55	1.52
4	B	673	NAG	C1-C2	2.41	1.55	1.52
4	D	673	NAG	C1-C2	2.60	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	672	NAG	C4-C3-C2	-3.19	106.26	111.23
4	A	672	NAG	C4-C3-C2	-2.73	106.99	111.23
4	D	673	NAG	C4-C3-C2	-2.69	107.05	111.23
4	D	671	NAG	O3-C3-C2	-2.63	103.91	109.11
4	C	673	NAG	O7-C7-C8	-2.47	117.52	122.06
4	A	673	NAG	O7-C7-C8	-2.18	118.06	122.06
4	A	671	NAG	C2-N2-C7	-2.10	120.34	123.04
4	A	671	NAG	C6-C5-C4	-2.09	107.86	113.02
4	C	673	NAG	C4-C3-C2	-2.06	108.03	111.23
4	C	673	NAG	O5-C5-C6	2.01	111.69	107.35
4	C	672	NAG	O5-C5-C6	2.20	112.12	107.35
4	C	673	NAG	O7-C7-N2	2.25	126.45	121.86
4	A	672	NAG	C3-C2-N2	2.33	116.13	110.56
4	A	672	NAG	O4-C4-C3	2.37	115.67	110.34
4	C	672	NAG	C2-N2-C7	2.42	126.15	123.04
4	B	672	NAG	C3-C2-N2	2.59	116.75	110.56
4	D	673	NAG	O3-C3-C2	2.70	114.47	109.11
4	A	673	NAG	C2-N2-C7	2.93	126.80	123.04
4	D	672	NAG	C3-C2-N2	2.99	117.72	110.56
4	D	672	NAG	C1-O5-C5	3.12	116.20	112.25
4	A	672	NAG	C1-O5-C5	3.21	116.33	112.25
4	A	672	NAG	C2-N2-C7	3.33	127.32	123.04
4	B	672	NAG	C2-N2-C7	3.40	127.41	123.04
4	B	673	NAG	C2-N2-C7	3.49	127.53	123.04
4	D	673	NAG	C2-N2-C7	4.26	128.52	123.04
4	D	671	NAG	C1-O5-C5	4.39	117.82	112.25
4	C	673	NAG	C1-O5-C5	5.03	118.63	112.25
4	B	673	NAG	C1-O5-C5	5.45	119.17	112.25
4	C	671	NAG	C1-O5-C5	5.83	119.65	112.25
4	A	673	NAG	C1-O5-C5	6.14	120.04	112.25
4	C	673	NAG	C2-N2-C7	6.53	131.43	123.04
4	D	673	NAG	C1-O5-C5	6.79	120.86	112.25
4	A	671	NAG	C1-O5-C5	9.16	123.88	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	672	NAG	1	0
4	D	673	NAG	1	0

## 5.6 Ligand geometry

18 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	605	1	30,50,50	2.25	6 (20%)	24,82,82	2.43	11 (45%)
3	NAG	A	661	1	14,14,15	0.84	1 (7%)	15,19,21	1.86	4 (26%)
3	NAG	A	681	1	14,14,15	0.54	0	15,19,21	0.90	0
6	416	A	701	-	19,23,23	0.93	0	27,37,37	0.98	1 (3%)
5	BOG	A	704	-	20,20,20	0.52	0	25,25,25	0.65	0
2	HEM	B	605	1	30,50,50	2.25	8 (26%)	24,82,82	2.24	11 (45%)
3	NAG	B	661	1	14,14,15	0.58	0	15,19,21	1.99	6 (40%)
3	NAG	B	681	1	14,14,15	0.56	0	15,19,21	0.78	0
6	416	B	701	-	19,23,23	0.88	0	27,37,37	1.10	2 (7%)
2	HEM	C	605	1	30,50,50	2.14	9 (30%)	24,82,82	2.38	11 (45%)
3	NAG	C	661	1	14,14,15	0.46	0	15,19,21	1.28	1 (6%)
3	NAG	C	681	1	14,14,15	0.70	0	15,19,21	1.05	1 (6%)
6	416	C	701	-	19,23,23	0.87	0	27,37,37	1.04	2 (7%)
5	BOG	C	703	-	20,20,20	0.52	0	25,25,25	0.94	1 (4%)
2	HEM	D	605	1	30,50,50	2.17	9 (30%)	24,82,82	2.35	12 (50%)
3	NAG	D	661	1	14,14,15	0.76	1 (7%)	15,19,21	2.36	4 (26%)
3	NAG	D	681	1	14,14,15	0.47	0	15,19,21	0.97	1 (6%)
6	416	D	701	-	19,23,23	0.98	1 (5%)	27,37,37	1.25	4 (14%)



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	605	1	-	0/10/54/54	0/0/8/8
3	NAG	A	661	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1
6	416	A	701	-	-	0/12/28/28	0/2/2/2
5	BOG	A	704	-	-	0/11/31/31	0/1/1/1
2	HEM	B	605	1	-	0/10/54/54	0/0/8/8
3	NAG	B	661	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	681	1	-	0/6/23/26	0/1/1/1
6	416	B	701	-	-	0/12/28/28	0/2/2/2
2	HEM	C	605	1	-	0/10/54/54	0/0/8/8
3	NAG	C	661	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	681	1	-	0/6/23/26	0/1/1/1
6	416	C	701	-	-	0/12/28/28	0/2/2/2
5	BOG	C	703	-	-	0/11/31/31	0/1/1/1
2	HEM	D	605	1	-	0/10/54/54	0/0/8/8
3	NAG	D	661	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	681	1	-	0/6/23/26	0/1/1/1
6	416	D	701	-	-	0/12/28/28	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-7.96	1.44	1.51
2	B	605	HEM	C3B-C4B	-7.29	1.45	1.51
2	D	605	HEM	C3B-C4B	-6.72	1.45	1.51
2	C	605	HEM	C3B-C4B	-6.28	1.46	1.51
2	B	605	HEM	C3D-C4D	-5.82	1.44	1.51
2	C	605	HEM	C3D-C4D	-5.23	1.44	1.51
2	D	605	HEM	C3D-C4D	-5.18	1.44	1.51
2	A	605	HEM	C3D-C4D	-5.01	1.45	1.51
2	A	605	HEM	C2C-C1C	-4.32	1.44	1.52
2	B	605	HEM	C2C-C1C	-3.81	1.45	1.52
2	D	605	HEM	C2C-C1C	-3.63	1.45	1.52
2	C	605	HEM	C2C-C1C	-3.56	1.45	1.52
2	C	605	HEM	C2D-C1D	-2.35	1.44	1.51
6	D	701	416	C8-C5	-2.04	1.51	1.54
2	D	605	HEM	C2B-C1B	-2.04	1.45	1.51
2	B	605	HEM	C2B-C1B	-2.01	1.45	1.51
2	C	605	HEM	C1C-NC	2.01	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	605	HEM	CAA-C2A	2.01	1.55	1.52
2	B	605	HEM	C1C-NC	2.06	1.38	1.36
2	A	605	HEM	C3C-CAC	2.07	1.55	1.51
2	B	605	HEM	C4C-NC	2.15	1.38	1.36
2	C	605	HEM	C4C-NC	2.18	1.38	1.36
2	D	605	HEM	C3C-CAC	2.24	1.55	1.51
2	C	605	HEM	C3C-CAC	2.25	1.55	1.51
2	D	605	HEM	FE-NC	2.40	2.05	1.95
3	D	661	NAG	C1-C2	2.41	1.55	1.52
2	D	605	HEM	C4C-NC	2.53	1.39	1.36
2	A	605	HEM	CAA-C2A	2.54	1.56	1.52
2	C	605	HEM	CAA-C2A	2.59	1.56	1.52
2	A	605	HEM	FE-NC	2.65	2.06	1.95
3	A	661	NAG	C1-C2	2.71	1.56	1.52
2	D	605	HEM	FE-ND	2.75	2.12	1.97
2	D	605	HEM	CAA-C2A	2.75	1.56	1.52
2	B	605	HEM	FE-NC	2.96	2.07	1.95
2	C	605	HEM	FE-NC	3.38	2.09	1.95

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	701	416	C3-C7-C12	-3.51	115.09	121.50
2	D	605	HEM	C3B-CAB-CBB	-2.89	120.03	124.46
6	B	701	416	C3-C7-C12	-2.81	116.37	121.50
2	A	605	HEM	CBD-CAD-C3D	-2.71	105.66	113.55
2	D	605	HEM	CMA-C3A-C4A	-2.70	123.89	128.36
3	A	661	NAG	C4-C3-C2	-2.70	107.03	111.23
2	B	605	HEM	C3B-CAB-CBB	-2.49	120.64	124.46
2	B	605	HEM	C3C-CAC-CBC	-2.38	120.81	124.46
2	C	605	HEM	CMA-C3A-C4A	-2.33	124.50	128.36
2	A	605	HEM	CMA-C3A-C4A	-2.31	124.55	128.36
2	B	605	HEM	CBD-CAD-C3D	-2.28	106.92	113.55
6	C	701	416	C3-C7-C12	-2.27	117.36	121.50
2	A	605	HEM	C3B-CAB-CBB	-2.26	120.99	124.46
6	A	701	416	C3-C7-C12	-2.25	117.39	121.50
2	C	605	HEM	C3B-CAB-CBB	-2.22	121.06	124.46
2	C	605	HEM	C3B-C4B-NB	-2.13	107.55	111.63
2	D	605	HEM	C3B-C4B-NB	-2.10	107.61	111.63
5	C	703	BOG	C4-C3-C2	-2.09	106.90	110.79
3	D	661	NAG	C4-C3-C2	-2.05	108.04	111.23
6	D	701	416	C1-C4-CL1	-2.04	115.35	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	HEM	C3B-C4B-NB	-2.04	107.73	111.63
3	B	661	NAG	C4-C3-C2	-2.03	108.07	111.23
6	C	701	416	C1-C4-CL1	-2.01	115.40	118.50
2	D	605	HEM	C2D-C3D-C4D	2.09	105.05	101.50
3	B	661	NAG	O5-C5-C6	2.19	112.10	107.35
6	D	701	416	O1-C6-C3	2.20	122.69	120.97
2	A	605	HEM	C3B-C4B-CHC	2.32	126.44	123.16
3	C	681	NAG	O5-C5-C6	2.33	112.40	107.35
3	A	661	NAG	O5-C5-C6	2.34	112.41	107.35
3	B	661	NAG	O3-C3-C2	2.34	113.76	109.11
3	D	681	NAG	C1-O5-C5	2.36	115.24	112.25
2	B	605	HEM	C3B-C4B-CHC	2.36	126.49	123.16
2	D	605	HEM	C2C-C1C-CHC	2.48	127.46	123.68
3	B	661	NAG	C3-C2-N2	2.49	116.51	110.56
2	B	605	HEM	CMD-C2D-C3D	2.50	125.41	114.35
2	A	605	HEM	C2D-C3D-C4D	2.51	105.75	101.50
2	C	605	HEM	C2C-C1C-CHC	2.52	127.52	123.68
2	D	605	HEM	CMD-C2D-C3D	2.61	125.87	114.35
6	B	701	416	O1-C6-C3	2.65	123.05	120.97
3	D	661	NAG	O5-C5-C6	2.69	113.18	107.35
2	D	605	HEM	C3B-C4B-CHC	2.74	127.02	123.16
6	D	701	416	C6-C3-C7	2.81	120.28	118.05
3	A	661	NAG	O3-C3-C2	2.84	114.75	109.11
2	B	605	HEM	C2D-C3D-C4D	2.88	106.39	101.50
2	C	605	HEM	CMD-C2D-C3D	2.89	127.12	114.35
3	B	661	NAG	C2-N2-C7	2.89	126.75	123.04
2	C	605	HEM	C3B-C4B-CHC	2.90	127.25	123.16
2	A	605	HEM	CMD-C2D-C3D	2.97	127.47	114.35
2	D	605	HEM	CMC-C2C-C3C	2.98	123.98	116.53
2	C	605	HEM	CMC-C2C-C3C	3.23	124.60	116.53
2	B	605	HEM	CMC-C2C-C3C	3.24	124.62	116.53
2	D	605	HEM	CAA-CBA-CGA	3.27	118.74	112.75
2	C	605	HEM	CAA-CBA-CGA	3.39	118.97	112.75
2	D	605	HEM	CMB-C2B-C3B	3.72	125.81	116.53
3	C	661	NAG	C1-O5-C5	3.84	117.12	112.25
2	A	605	HEM	CAD-C3D-C4D	3.86	126.08	112.47
2	A	605	HEM	CMB-C2B-C3B	3.87	126.19	116.53
2	B	605	HEM	CMB-C2B-C3B	3.88	126.21	116.53
2	A	605	HEM	CAA-CBA-CGA	3.97	120.03	112.75
2	C	605	HEM	CMB-C2B-C3B	3.98	126.46	116.53
2	B	605	HEM	CAD-C3D-C4D	4.08	126.86	112.47
2	A	605	HEM	CMC-C2C-C3C	4.09	126.75	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	605	HEM	CAD-C3D-C4D	4.17	127.19	112.47
3	D	661	NAG	C2-N2-C7	4.20	128.44	123.04
2	C	605	HEM	CAD-C3D-C4D	4.43	128.09	112.47
2	B	605	HEM	CAD-C3D-C2D	4.70	126.73	113.22
3	B	661	NAG	C1-O5-C5	4.71	118.22	112.25
2	C	605	HEM	CAD-C3D-C2D	4.82	127.08	113.22
3	A	661	NAG	C1-O5-C5	4.87	118.43	112.25
2	D	605	HEM	CAD-C3D-C2D	5.06	127.76	113.22
2	A	605	HEM	CAD-C3D-C2D	5.18	128.12	113.22
3	D	661	NAG	C1-O5-C5	6.65	120.68	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	661	NAG	C1
3	A	661	NAG	C1
3	C	661	NAG	C1
3	D	661	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	2	0
6	A	701	416	2	0
2	B	605	HEM	1	0
6	B	701	416	2	0
2	C	605	HEM	1	0
6	C	701	416	1	0
6	D	701	416	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/587 (94%)	-0.40	1 (0%) 95 94	29, 47, 64, 79	0
1	B	552/587 (94%)	-0.40	3 (0%) 91 88	26, 46, 64, 76	0
1	C	552/587 (94%)	-0.28	6 (1%) 82 74	35, 54, 74, 88	0
1	D	552/587 (94%)	-0.33	4 (0%) 89 84	35, 53, 71, 82	0
All	All	2208/2348 (94%)	-0.35	14 (0%) 90 86	26, 50, 69, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	ALA	4.6
1	B	59	PHE	4.3
1	D	59	PHE	3.4
1	D	354	ASN	3.4
1	D	63	ILE	3.0
1	B	60	LEU	2.7
1	C	385	ASP	2.6
1	C	200	HIS	2.6
1	C	55	THR	2.4
1	A	64	LYS	2.4
1	D	60	LEU	2.3
1	C	83	GLY	2.3
1	C	371	TYR	2.1
1	B	201	LYS	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 ⓘ

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	NAG	A	671	14/15	0.90	0.25	1.56	33,36,38,40	0
4	NAG	C	671	14/15	0.91	0.23	1.49	37,39,42,46	0
4	NAG	D	671	14/15	0.93	0.17	0.62	32,34,37,40	0
4	NAG	B	671	14/15	0.94	0.18	0.36	27,34,36,40	0
4	NAG	A	673	14/15	0.81	0.39	-	51,53,53,54	0
4	NAG	C	673	14/15	0.66	0.48	-	60,62,63,64	0
4	NAG	C	672	14/15	0.91	0.34	-	49,51,53,57	0
4	NAG	A	672	14/15	0.91	0.30	-	34,40,43,47	0
4	NAG	B	672	14/15	0.90	0.32	-	42,45,46,49	0
4	NAG	B	673	14/15	0.82	0.45	-	52,53,56,57	0
4	NAG	D	673	14/15	0.67	0.45	-	49,52,53,54	0
4	NAG	D	672	14/15	0.89	0.31	-	44,46,47,48	0

### 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
3	NAG	D	681	14/15	0.89	0.37	4.59	43,44,46,46	0
3	NAG	B	681	14/15	0.91	0.43	3.32	44,46,47,48	0
3	NAG	A	681	14/15	0.80	0.35	3.02	49,52,53,54	0
3	NAG	C	661	14/15	0.88	0.38	2.20	35,39,42,42	0
6	416	A	701	22/22	0.94	0.18	-0.08	49,52,53,53	0
2	HEM	A	605	43/43	0.93	0.17	-0.28	24,32,39,41	0
2	HEM	C	605	43/43	0.94	0.16	-0.38	29,33,38,40	0
2	HEM	D	605	43/43	0.93	0.17	-0.42	32,35,44,47	0
6	416	D	701	22/22	0.94	0.18	-0.52	52,55,56,58	0
6	416	B	701	22/22	0.96	0.17	-0.60	49,52,55,57	0
6	416	C	701	22/22	0.94	0.16	-0.68	55,59,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BOG	C	703	20/20	0.95	0.14	-0.71	55,56,58,58	0
2	HEM	B	605	43/43	0.95	0.15	-0.72	31,32,38,41	0
5	BOG	A	704	20/20	0.96	0.13	-0.79	39,41,44,44	0
3	NAG	A	661	14/15	0.81	0.34	-	31,36,39,40	0
3	NAG	C	681	14/15	0.72	0.38	-	54,57,58,58	0
3	NAG	D	661	14/15	0.83	0.35	-	34,37,38,38	0
3	NAG	B	661	14/15	0.84	0.43	-	36,39,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.