Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:04 AM GMT

PDB ID	:	3NTB
Title	:	Structure of 6-methylthio naproxen analog bound to mCOX-2.
Authors	:	Duggan, K.C.; Musee, J.; Walters, M.J.; Harp, J.M.; Kiefer, J.R.; Oates, J.A.; Marnett, L.J.
Deposited on	:	2010-07-03
Resolution	:	2.27 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

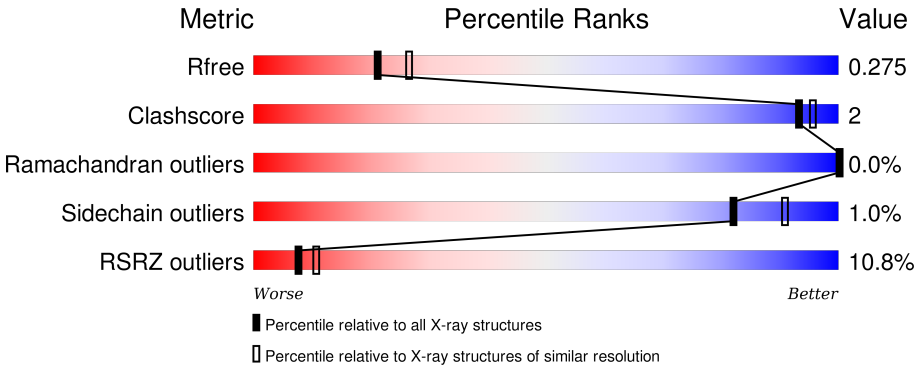
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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 >=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 <=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	11% 89% 5% 6%
1	B	587	12% 88% 6% 6%
1	C	587	9% 88% 6% 6%
1	D	587	9% 88% 6% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	661	X	-	-	-
3	NAG	A	681	-	-	-	X
3	NAG	B	661	X	-	-	X
3	NAG	C	661	X	-	-	-
3	NAG	C	681	-	-	-	X
3	NAG	D	661	X	-	-	-
5	BOG	A	7	-	-	-	X
5	BOG	D	8	-	-	-	X

2 Entry composition

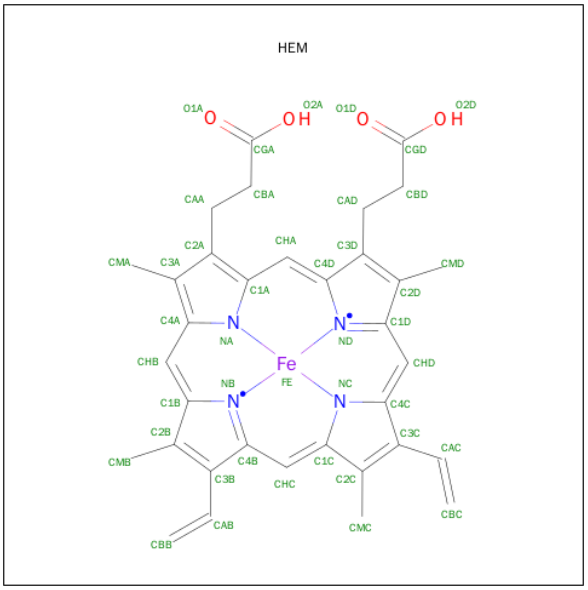
There are 7 unique types of molecules in this entry. The entry contains 19636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-endoperoxide 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	551	Total	C	N	O	S	0	0	0
			4465	2880	748	812	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	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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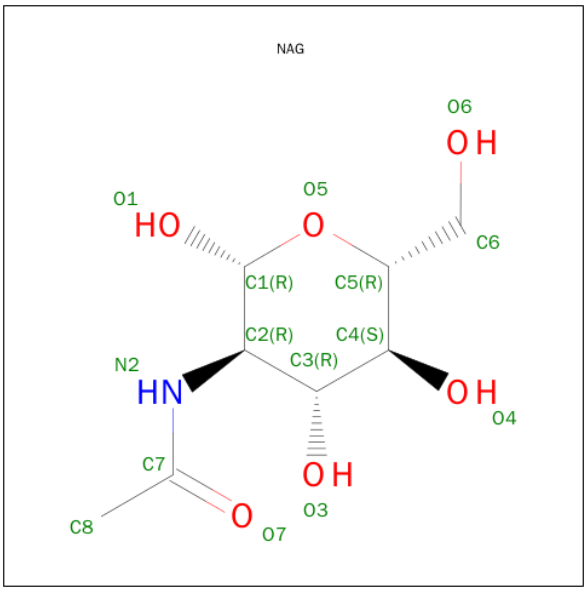
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

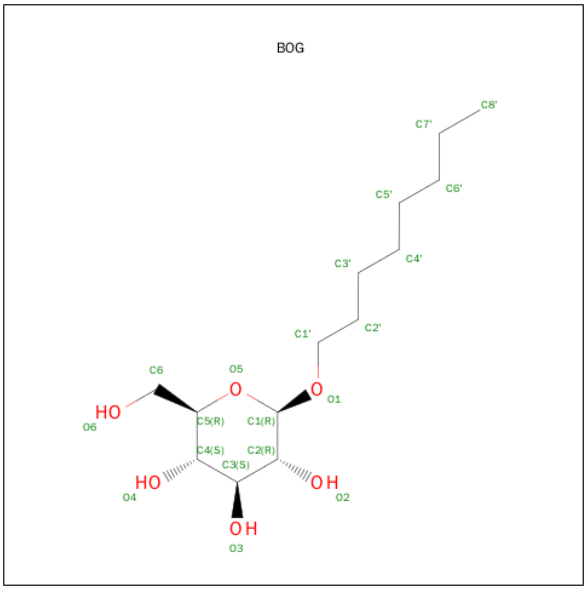


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	C	1	Total	C	N	O		0	0
			14	8	1	5			
3	C	1	Total	C	N	O		0	0
			14	8	1	5			
3	D	1	Total	C	N	O		0	0
			14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

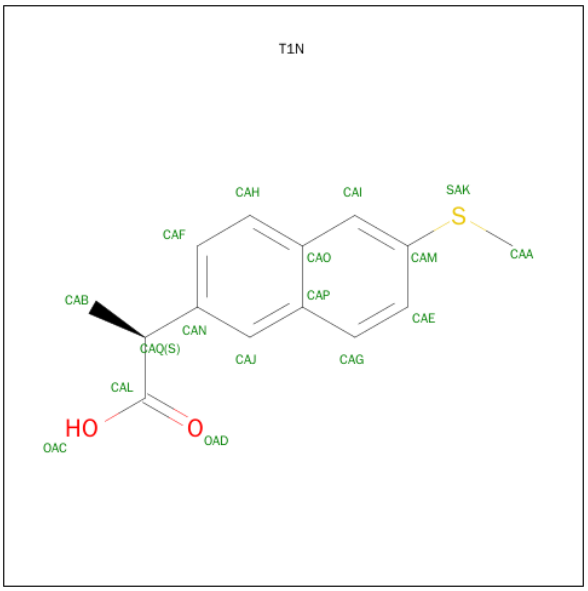
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total C N O 42 24 3 15	0	0
4	B	3	Total C N O 42 24 3 15	0	0
4	C	3	Total C N O 42 24 3 15	0	0
4	D	3	Total C N O 42 24 3 15	0	0

- 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 20 14 6	0	0
5	A	1	Total C O 20 14 6	0	0
5	B	1	Total C O 20 14 6	0	0
5	C	1	Total C O 20 14 6	0	0
5	D	1	Total C O 20 14 6	0	0
5	D	1	Total C O 20 14 6	0	0

- Molecule 6 is (2S)-2-[6-(METHYLSULFANYL)NAPHTHALEN-2-YL]PROPANOIC ACID (three-letter code: T1N) (formula: $C_{14}H_{14}O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 17 14 2 1	0	0
6	B	1	Total C O S 17 14 2 1	0	0
6	C	1	Total C O S 17 14 2 1	0	0
6	D	1	Total C O S 17 14 2 1	0	0

- Molecule 7 is water.

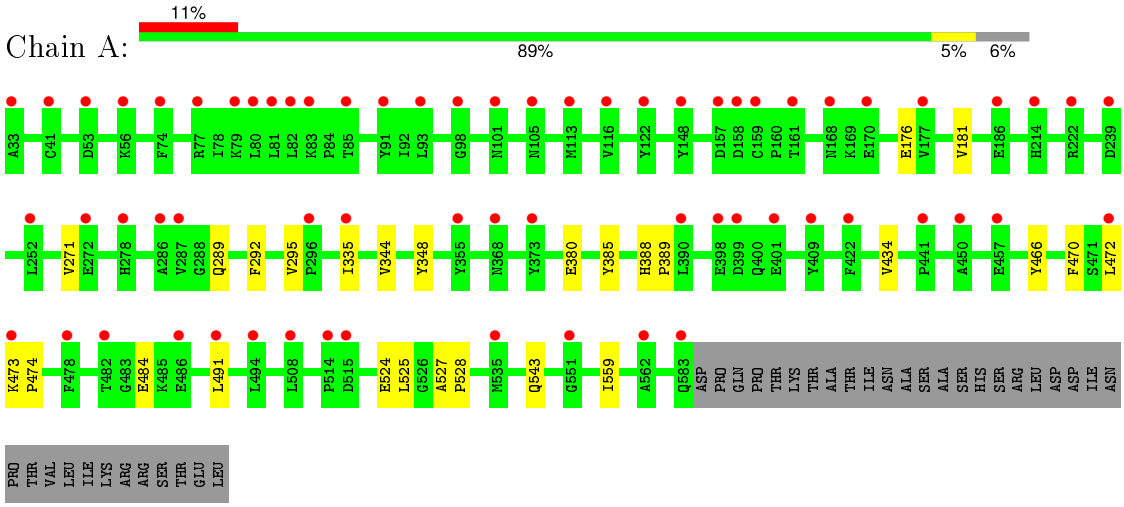
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	278	Total O 278 278	0	0
7	B	245	Total O 245 245	0	0
7	C	291	Total O 291 291	0	0
7	D	295	Total O 295 295	0	0

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.

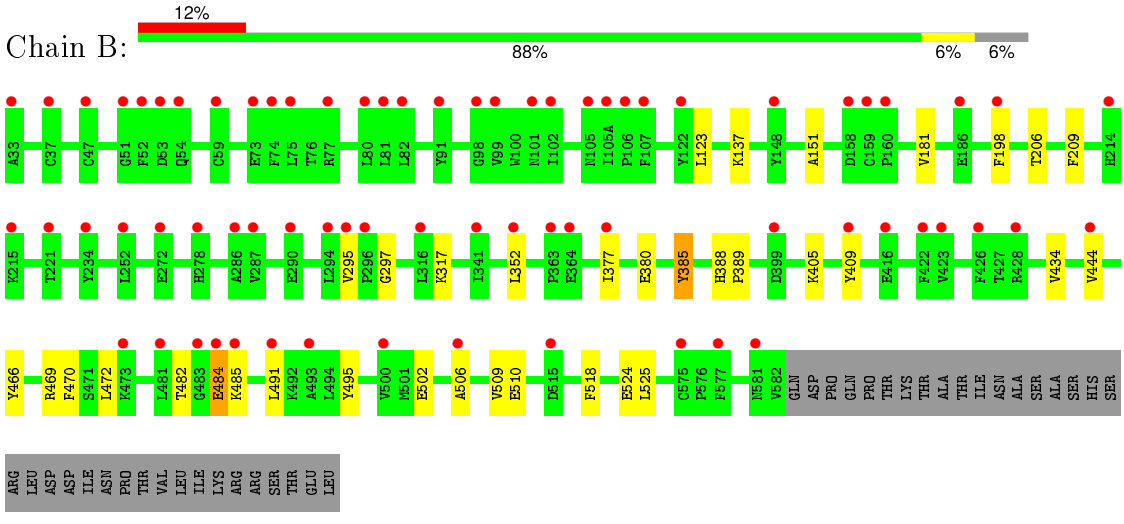
- Molecule 1: Prostaglandin-endoperoxide synthase 2

Chain A:



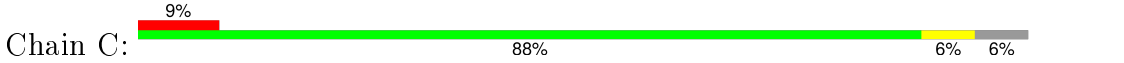
- Molecule 1: Prostaglandin-endoperoxide synthase 2

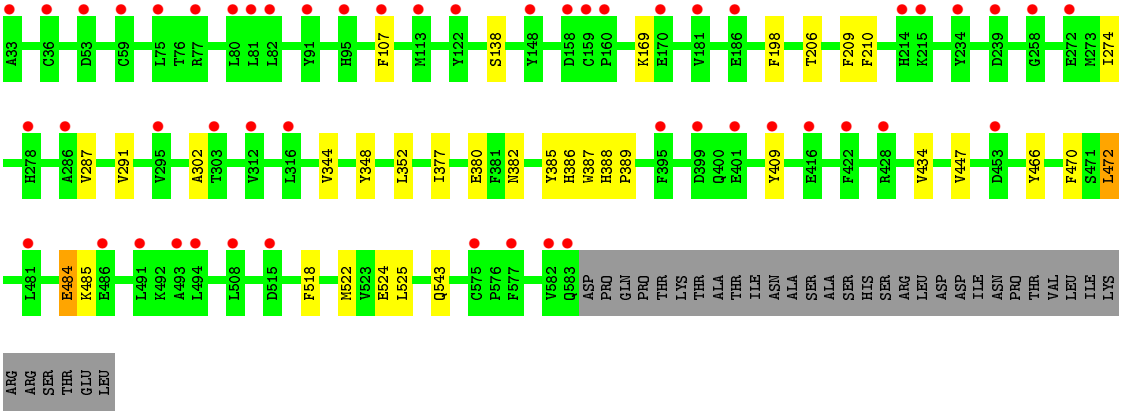
Chain B:



- Molecule 1: Prostaglandin-endoperoxide synthase 2

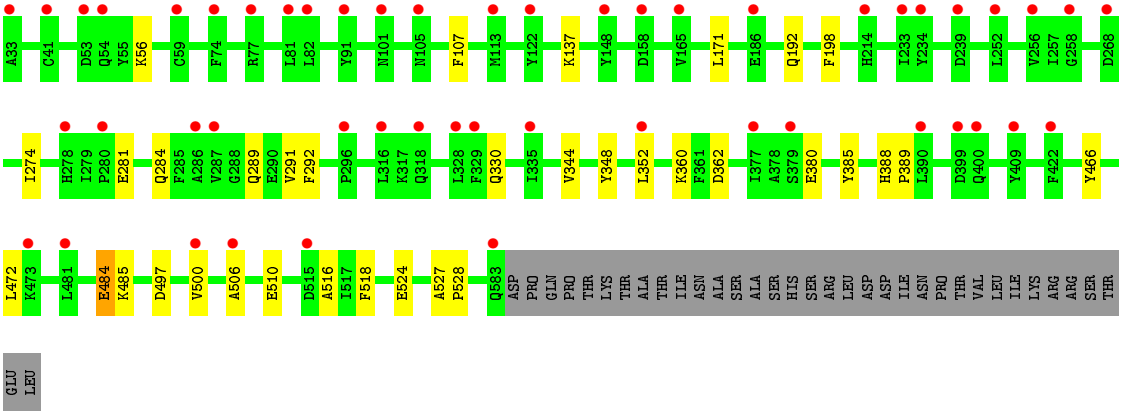
Chain C:





- Molecule 1: Prostaglandin-endoperoxide synthase 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	181.20Å 134.22Å 121.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.48 – 2.27 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.48-2.27) 96.7 (19.94-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.266 0.242 , 0.275	Depositor DCC
R_{free} test set	13522 reflections (11.17%)	DCC
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	5 of 145666 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19636	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 50.01 % 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 6.8750e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, T1N, 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	0.34	0/4601	0.47	0/6239
1	B	0.34	0/4592	0.46	0/6227
1	C	0.34	0/4601	0.47	0/6239
1	D	0.34	0/4601	0.46	0/6239
All	All	0.34	0/18395	0.47	0/24944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4373	12	0
1	B	4465	0	4365	21	0
1	C	4474	0	4373	20	0
1	D	4474	0	4373	18	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	2	0
2	D	43	0	30	0	0
3	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
5	A	40	0	56	0	0
5	B	20	0	28	0	0
5	C	20	0	28	0	0
5	D	40	0	56	0	0
6	A	17	0	13	0	0
6	B	17	0	13	0	0
6	C	17	0	13	0	0
6	D	17	0	13	0	0
7	A	278	0	0	0	0
7	B	245	0	0	0	0
7	C	291	0	0	0	0
7	D	295	0	0	0	0
All	All	19636	0	18076	68	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 2.

All (68) 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:472:LEU:HD21	1:A:524:GLU:HG3	1.82	0.60
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.38	0.58
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.39	0.58
1:D:198:PHE:HZ	1:D:352:LEU:HD13	1.69	0.57
1:B:352:LEU:HD11	1:B:518:PHE:HE2	1.71	0.55
1:C:447:VAL:HG13	2:C:619:HEM:HBA1	1.88	0.55
1:B:123:LEU:O	1:B:469:ARG:NH2	2.40	0.55
1:B:151:ALA:O	1:B:469:ARG:NH1	2.40	0.54
1:C:352:LEU:HD22	1:C:518:PHE:HE2	1.72	0.54
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.88	0.54
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.44	0.53
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.44	0.52
1:C:382:ASN:O	1:C:386:HIS:HD2	1.93	0.52
1:C:484:GLU:HG2	1:C:485:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.45	0.51
1:D:472:LEU:HD11	1:D:524:GLU:HG3	1.91	0.51
1:C:472:LEU:HD11	1:C:524:GLU:HG3	1.94	0.49
1:B:209:PHE:HB2	1:B:377:ILE:HG13	1.95	0.49
1:C:198:PHE:HZ	1:C:352:LEU:HD21	1.77	0.48
1:D:281:GLU:HA	1:D:284:GLN:HE21	1.79	0.48
1:C:543:GLN:O	1:D:137:LYS:HE2	2.13	0.48
1:A:470:PHE:CD2	1:A:525:LEU:HD22	2.48	0.48
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.95	0.48
1:C:209:PHE:HB2	1:C:377:ILE:HG13	1.96	0.48
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.95	0.47
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.51	0.46
1:A:543:GLN:O	1:B:137:LYS:HE2	2.16	0.46
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.51	0.46
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.99	0.45
1:C:484:GLU:HG2	1:C:485:LYS:N	2.31	0.45
1:B:295:VAL:HG12	1:B:297:GLY:H	1.81	0.45
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.98	0.45
1:C:470:PHE:CD2	1:C:525:LEU:HD22	2.52	0.44
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.99	0.44
1:D:506:ALA:O	1:D:510:GLU:HB2	2.17	0.44
1:A:181:VAL:HG21	1:A:491:LEU:HD21	1.99	0.44
1:D:527:ALA:HB3	1:D:528:PRO:HD3	2.01	0.43
1:C:206:THR:HB	1:C:210:PHE:CD2	2.53	0.43
1:B:181:VAL:HG21	1:B:491:LEU:HD21	2.00	0.43
1:C:138:SER:HB2	1:D:330:GLN:HB3	2.00	0.43
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.54	0.43
1:C:388:HIS:N	1:C:389:PRO:CD	2.81	0.43
1:C:387:TRP:HB2	2:C:619:HEM:HAC	2.01	0.43
1:B:482:THR:HG22	1:B:509:VAL:HG12	1.99	0.43
1:D:344:VAL:HA	1:D:348:TYR:HB3	2.00	0.43
1:D:497:ASP:HB3	1:D:500:VAL:HG23	2.01	0.43
1:B:388:HIS:N	1:B:389:PRO:CD	2.82	0.43
1:C:274:ILE:HD12	1:C:291:VAL:HG12	2.02	0.42
1:B:484:GLU:HG2	1:B:485:LYS:H	1.84	0.42
1:B:506:ALA:O	1:B:510:GLU:HB2	2.20	0.42
1:D:289:GLN:HG2	1:D:292:PHE:CE1	2.55	0.41
1:D:388:HIS:N	1:D:389:PRO:CD	2.83	0.41
1:D:484:GLU:HG2	1:D:485:LYS:H	1.85	0.41
1:C:344:VAL:HA	1:C:348:TYR:HB3	2.01	0.41
1:A:388:HIS:N	1:A:389:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HA	1:A:559:ILE:HD11	2.02	0.41
1:D:352:LEU:HD11	1:D:518:PHE:CE2	2.56	0.41
1:B:470:PHE:CD2	1:B:525:LEU:HD22	2.56	0.41
1:B:495:TYR:HE1	1:B:502:GLU:HG3	1.85	0.41
1:A:473:LYS:HA	1:A:474:PRO:HD3	1.96	0.41
1:D:360:LYS:HE3	1:D:362:ASP:HB2	2.03	0.41
1:B:198:PHE:HZ	1:B:352:LEU:HD13	1.86	0.41
1:C:287:VAL:HG11	1:C:302:ALA:HB1	2.02	0.40
1:B:206:THR:HG21	1:B:385:TYR:CE2	2.56	0.40
1:D:274:ILE:HD12	1:D:291:VAL:HG12	2.03	0.40
1:C:518:PHE:HB3	1:C:522:MET:HB3	2.03	0.40
1:D:192:GLN:HG3	1:D:516:ALA:HA	2.04	0.40
1:B:444:VAL:HG12	1:B:444:VAL:O	2.22	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%)	536 (98%)	14 (2%)	0	100	100
1	B	549/587 (94%)	534 (97%)	14 (3%)	1 (0%)	52	63
1	C	550/587 (94%)	537 (98%)	13 (2%)	0	100	100
1	D	550/587 (94%)	534 (97%)	16 (3%)	0	100	100
All	All	2199/2348 (94%)	2141 (97%)	57 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	409	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	493/525 (94%)	488 (99%)	5 (1%)	82 91
1	B	492/525 (94%)	488 (99%)	4 (1%)	86 93
1	C	493/525 (94%)	487 (99%)	6 (1%)	78 88
1	D	493/525 (94%)	488 (99%)	5 (1%)	82 91
All	All	1971/2100 (94%)	1951 (99%)	20 (1%)	82 91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLU
1	A	271	VAL
1	A	295	VAL
1	A	385	TYR
1	A	484	GLU
1	B	317	LYS
1	B	385	TYR
1	B	405	LYS
1	B	484	GLU
1	C	107	PHE
1	C	169	LYS
1	C	385	TYR
1	C	409	TYR
1	C	472	LEU
1	C	484	GLU
1	D	56	LYS
1	D	107	PHE
1	D	171	LEU
1	D	385	TYR
1	D	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	C	369	GLN
1	C	386	HIS
1	C	583	GLN
1	D	284	GLN
1	D	369	GLN
1	D	386	HIS

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	0.47	0	15,19,21	0.95	1 (6%)
4	NAG	A	672	4	14,14,15	0.48	0	15,19,21	1.62	5 (33%)
4	NAG	A	673	4	14,14,15	0.61	0	15,19,21	1.08	1 (6%)
4	NAG	B	671	1,4	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
4	NAG	B	672	4	14,14,15	0.48	0	15,19,21	1.02	1 (6%)
4	NAG	B	673	4	14,14,15	0.52	0	15,19,21	1.74	2 (13%)
4	NAG	C	671	1,4	14,14,15	0.48	0	15,19,21	0.90	1 (6%)
4	NAG	C	672	4	14,14,15	0.51	0	15,19,21	1.14	1 (6%)
4	NAG	C	673	4	14,14,15	0.50	0	15,19,21	1.61	2 (13%)
4	NAG	D	671	1,4	14,14,15	0.47	0	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	672	4	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
4	NAG	D	673	4	14,14,15	0.55	0	15,19,21	1.97	3 (20%)

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	672	NAG	O4-C4-C3	-2.32	105.12	110.34
4	D	673	NAG	O5-C5-C6	2.06	111.81	107.35
4	C	673	NAG	O5-C5-C6	2.07	111.82	107.35
4	A	672	NAG	C4-C3-C2	2.10	114.49	111.23
4	A	672	NAG	C3-C4-C5	2.27	114.16	110.20
4	A	671	NAG	C1-O5-C5	2.53	115.46	112.25
4	B	671	NAG	C1-O5-C5	2.55	115.48	112.25
4	A	672	NAG	C1-O5-C5	2.57	115.51	112.25
4	B	673	NAG	C2-N2-C7	2.59	126.37	123.04
4	C	671	NAG	C1-O5-C5	2.72	115.71	112.25
4	D	673	NAG	C2-N2-C7	2.74	126.56	123.04
4	D	671	NAG	C1-O5-C5	2.78	115.78	112.25
4	D	672	NAG	C2-N2-C7	2.81	126.65	123.04
4	A	673	NAG	C2-N2-C7	2.88	126.74	123.04
4	B	672	NAG	C2-N2-C7	3.01	126.91	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	672	NAG	C2-N2-C7	3.23	127.18	123.04
4	C	672	NAG	C2-N2-C7	3.28	127.25	123.04
4	C	673	NAG	C1-O5-C5	5.00	118.60	112.25
4	B	673	NAG	C1-O5-C5	5.48	119.20	112.25
4	D	673	NAG	C1-O5-C5	6.25	120.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

22 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	$\#\|Z\| > 2$
6	T1N	A	3	-	15,18,18	1.04	0	21,25,25	1.07	1 (4%)
2	HEM	A	619	1	30,50,50	2.17	9 (30%)	24,82,82	2.32	10 (41%)
3	NAG	A	661	1	14,14,15	0.46	0	15,19,21	1.23	1 (6%)
3	NAG	A	681	1	14,14,15	0.48	0	15,19,21	0.72	0
5	BOG	A	7	-	20,20,20	0.50	0	25,25,25	0.54	0
5	BOG	A	703	-	20,20,20	0.48	0	25,25,25	0.59	0
6	T1N	B	1	-	15,18,18	1.04	0	21,25,25	0.91	0
5	BOG	B	6	-	20,20,20	0.46	0	25,25,25	0.62	0
2	HEM	B	619	1,7	30,50,50	2.18	11 (36%)	24,82,82	2.35	12 (50%)
3	NAG	B	661	1	14,14,15	0.50	0	15,19,21	1.70	2 (13%)
3	NAG	B	681	1	14,14,15	0.52	0	15,19,21	0.73	0
6	T1N	C	2	-	15,18,18	1.05	0	21,25,25	0.98	1 (4%)
5	BOG	C	5	-	20,20,20	0.46	0	25,25,25	0.58	0
2	HEM	C	619	1	30,50,50	2.19	9 (30%)	24,82,82	2.31	10 (41%)
3	NAG	C	661	1	14,14,15	0.45	0	15,19,21	1.24	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	681	1	14,14,15	0.56	0	15,19,21	1.23	2 (13%)
6	T1N	D	4	-	15,18,18	1.04	0	21,25,25	1.02	1 (4%)
2	HEM	D	619	1	30,50,50	2.14	7 (23%)	24,82,82	2.35	10 (41%)
3	NAG	D	661	1	14,14,15	0.46	0	15,19,21	1.09	1 (6%)
3	NAG	D	681	1	14,14,15	0.50	0	15,19,21	0.73	0
5	BOG	D	703	-	20,20,20	0.49	0	25,25,25	0.62	0
5	BOG	D	8	-	20,20,20	0.48	0	25,25,25	0.59	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
6	T1N	A	3	-	-	0/6/10/10	0/2/2/2
2	HEM	A	619	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
5	BOG	A	7	-	-	0/11/31/31	0/1/1/1
5	BOG	A	703	-	-	0/11/31/31	0/1/1/1
6	T1N	B	1	-	-	0/6/10/10	0/2/2/2
5	BOG	B	6	-	-	0/11/31/31	0/1/1/1
2	HEM	B	619	1,7	-	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	T1N	C	2	-	-	0/6/10/10	0/2/2/2
5	BOG	C	5	-	-	0/11/31/31	0/1/1/1
2	HEM	C	619	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	T1N	D	4	-	-	0/6/10/10	0/2/2/2
2	HEM	D	619	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
5	BOG	D	703	-	-	0/11/31/31	0/1/1/1
5	BOG	D	8	-	-	0/11/31/31	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	619	HEM	C3B-C4B	-6.89	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	619	HEM	C3B-C4B	-6.89	1.45	1.51
2	B	619	HEM	C3B-C4B	-6.83	1.45	1.51
2	D	619	HEM	C3B-C4B	-6.74	1.45	1.51
2	C	619	HEM	C3D-C4D	-5.28	1.44	1.51
2	D	619	HEM	C3D-C4D	-5.18	1.44	1.51
2	B	619	HEM	C3D-C4D	-5.12	1.45	1.51
2	A	619	HEM	C3D-C4D	-5.02	1.45	1.51
2	A	619	HEM	C2C-C1C	-3.71	1.45	1.52
2	B	619	HEM	C2C-C1C	-3.68	1.45	1.52
2	D	619	HEM	C2C-C1C	-3.66	1.45	1.52
2	C	619	HEM	C2C-C1C	-3.66	1.45	1.52
2	A	619	HEM	C2D-C1D	-2.06	1.45	1.51
2	C	619	HEM	C2D-C1D	-2.04	1.45	1.51
2	B	619	HEM	C2D-C1D	-2.02	1.45	1.51
2	D	619	HEM	C4C-NC	2.01	1.38	1.36
2	B	619	HEM	C4C-NC	2.01	1.38	1.36
2	A	619	HEM	C3C-CAC	2.03	1.55	1.51
2	A	619	HEM	C4C-NC	2.04	1.38	1.36
2	A	619	HEM	C1C-NC	2.08	1.38	1.36
2	B	619	HEM	CAA-C2A	2.09	1.55	1.52
2	B	619	HEM	C3B-CAB	2.11	1.55	1.51
2	B	619	HEM	C3C-CAC	2.12	1.55	1.51
2	C	619	HEM	C3C-CAC	2.12	1.55	1.51
2	C	619	HEM	C1C-NC	2.15	1.38	1.36
2	C	619	HEM	FE-ND	2.16	2.08	1.97
2	D	619	HEM	C1C-NC	2.16	1.38	1.36
2	D	619	HEM	FE-ND	2.20	2.09	1.97
2	B	619	HEM	C1C-NC	2.25	1.38	1.36
2	A	619	HEM	FE-ND	2.32	2.09	1.97
2	C	619	HEM	CAA-C2A	2.33	1.56	1.52
2	B	619	HEM	FE-ND	2.41	2.10	1.97
2	B	619	HEM	FE-NC	2.45	2.05	1.95
2	D	619	HEM	FE-NC	2.56	2.05	1.95
2	C	619	HEM	FE-NC	2.64	2.06	1.95
2	A	619	HEM	FE-NC	2.83	2.06	1.95

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	619	HEM	C3B-CAB-CBB	-2.85	120.08	124.46
2	A	619	HEM	C3B-CAB-CBB	-2.81	120.15	124.46
2	C	619	HEM	C3B-CAB-CBB	-2.77	120.21	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	619	HEM	CBA-CAA-C2A	-2.76	107.58	112.53
2	D	619	HEM	C3C-CAC-CBC	-2.75	120.24	124.46
6	A	3	T1N	CAL-CAQ-CAN	-2.60	107.21	112.32
2	A	619	HEM	C3C-CAC-CBC	-2.56	120.52	124.46
6	D	4	T1N	CAL-CAQ-CAN	-2.56	107.29	112.32
2	B	619	HEM	C3B-CAB-CBB	-2.47	120.66	124.46
2	B	619	HEM	C3C-CAC-CBC	-2.45	120.70	124.46
6	C	2	T1N	CAL-CAQ-CAN	-2.33	107.75	112.32
2	D	619	HEM	C3B-C4B-NB	-2.12	107.58	111.63
2	C	619	HEM	C3B-C4B-NB	-2.11	107.59	111.63
2	A	619	HEM	C3B-C4B-NB	-2.07	107.67	111.63
2	C	619	HEM	C3C-CAC-CBC	-2.07	121.29	124.46
2	B	619	HEM	C3B-C4B-NB	-2.06	107.69	111.63
2	B	619	HEM	C2C-C1C-CHC	2.00	126.73	123.68
2	B	619	HEM	C2D-C3D-C4D	2.31	105.42	101.50
2	D	619	HEM	C2D-C3D-C4D	2.44	105.64	101.50
2	A	619	HEM	C2D-C3D-C4D	2.50	105.73	101.50
2	C	619	HEM	C2D-C3D-C4D	2.50	105.74	101.50
2	A	619	HEM	C3B-C4B-CHC	2.51	126.70	123.16
2	C	619	HEM	C3B-C4B-CHC	2.67	126.92	123.16
2	D	619	HEM	C3B-C4B-CHC	2.71	126.98	123.16
2	B	619	HEM	C3B-C4B-CHC	2.74	127.02	123.16
3	C	681	NAG	C4-C3-C2	2.82	115.62	111.23
2	A	619	HEM	CMD-C2D-C3D	2.87	127.02	114.35
2	D	619	HEM	CMD-C2D-C3D	2.88	127.08	114.35
2	C	619	HEM	CMD-C2D-C3D	2.89	127.13	114.35
2	B	619	HEM	CMD-C2D-C3D	2.91	127.24	114.35
3	C	681	NAG	C3-C4-C5	2.92	115.28	110.20
3	D	661	NAG	C1-O5-C5	3.38	116.54	112.25
3	B	661	NAG	C2-N2-C7	3.43	127.44	123.04
2	A	619	HEM	CMB-C2B-C3B	3.82	126.07	116.53
2	C	619	HEM	CMB-C2B-C3B	3.84	126.13	116.53
2	C	619	HEM	CMC-C2C-C3C	3.85	126.13	116.53
2	D	619	HEM	CMC-C2C-C3C	3.85	126.14	116.53
2	B	619	HEM	CMC-C2C-C3C	3.85	126.14	116.53
2	A	619	HEM	CMC-C2C-C3C	3.86	126.17	116.53
2	D	619	HEM	CMB-C2B-C3B	3.91	126.30	116.53
2	B	619	HEM	CMB-C2B-C3B	3.97	126.45	116.53
2	C	619	HEM	CAD-C3D-C4D	4.07	126.83	112.47
2	D	619	HEM	CAD-C3D-C4D	4.07	126.83	112.47
3	A	661	NAG	C1-O5-C5	4.11	117.46	112.25
2	B	619	HEM	CAD-C3D-C4D	4.11	126.96	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	661	NAG	C1-O5-C5	4.11	117.46	112.25
2	A	619	HEM	CAD-C3D-C4D	4.14	127.07	112.47
3	B	661	NAG	C1-O5-C5	4.71	118.23	112.25
2	A	619	HEM	CAD-C3D-C2D	4.86	127.19	113.22
2	C	619	HEM	CAD-C3D-C2D	4.95	127.43	113.22
2	D	619	HEM	CAD-C3D-C2D	4.98	127.52	113.22
2	B	619	HEM	CAD-C3D-C2D	5.01	127.62	113.22

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	619	HEM	2	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^{th} 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^2)	Q<0.9
1	A	552/587 (94%)	0.83	65 (11%) 6 9	35, 49, 69, 84	0
1	B	551/587 (93%)	0.89	71 (12%) 5 7	36, 52, 75, 89	0
1	C	552/587 (94%)	0.74	52 (9%) 11 15	34, 47, 63, 77	0
1	D	552/587 (94%)	0.73	50 (9%) 11 16	35, 47, 62, 75	0
All	All	2207/2348 (93%)	0.80	238 (10%) 8 11	34, 48, 68, 89	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	TYR	10.0
1	C	583	GLN	7.5
1	C	80	LEU	6.8
1	D	122	TYR	5.5
1	B	33	ALA	5.5
1	B	122	TYR	5.4
1	B	74	PHE	5.0
1	C	486	GLU	4.6
1	B	481	LEU	4.4
1	A	278	HIS	4.4
1	A	81	LEU	4.3
1	A	494	LEU	4.3
1	A	122	TYR	4.2
1	D	287	VAL	4.1
1	A	101	ASN	4.1
1	A	177	VAL	4.1
1	D	296	PRO	4.1
1	C	122	TYR	4.1
1	B	53	ASP	4.0
1	B	82	LEU	4.0
1	B	81	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	422	PHE	3.9
1	D	81	LEU	3.9
1	D	422	PHE	3.8
1	A	161	THR	3.7
1	C	181	VAL	3.7
1	B	422	PHE	3.7
1	A	77	ARG	3.7
1	B	399	ASP	3.6
1	D	158	ASP	3.6
1	D	82	LEU	3.6
1	B	473	LYS	3.6
1	D	399	ASP	3.6
1	A	105	ASN	3.6
1	D	105	ASN	3.6
1	B	105(A)	ILE	3.6
1	B	215	LYS	3.6
1	C	278	HIS	3.6
1	B	364	GLU	3.5
1	C	91	TYR	3.5
1	B	158	ASP	3.5
1	B	54	GLN	3.5
1	A	91	TYR	3.5
1	D	280	PRO	3.5
1	D	278	HIS	3.5
1	D	53	ASP	3.4
1	A	422	PHE	3.4
1	D	101	ASN	3.3
1	A	80	LEU	3.3
1	C	399	ASP	3.3
1	A	583	GLN	3.3
1	C	493	ALA	3.3
1	C	577	PHE	3.3
1	A	457	GLU	3.3
1	B	148	TYR	3.3
1	D	77	ARG	3.3
1	B	287	VAL	3.3
1	C	75	LEU	3.3
1	C	312	VAL	3.3
1	D	286	ALA	3.3
1	A	239	ASP	3.3
1	B	577	PHE	3.2
1	B	214	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	484	GLU	3.2
1	B	316	LEU	3.2
1	A	33	ALA	3.2
1	B	483	GLY	3.2
1	A	401	GLU	3.2
1	B	377	ILE	3.2
1	C	160	PRO	3.2
1	B	296	PRO	3.2
1	A	158	ASP	3.1
1	D	481	LEU	3.1
1	A	74	PHE	3.1
1	A	159	CYS	3.1
1	B	278	HIS	3.1
1	B	286	ALA	3.1
1	D	318	GLN	3.0
1	B	160	PRO	3.0
1	C	272	GLU	3.0
1	A	82	LEU	3.0
1	B	105	ASN	3.0
1	A	409	TYR	3.0
1	C	148	TYR	3.0
1	A	472	LEU	3.0
1	C	494	LEU	3.0
1	D	252	LEU	2.9
1	A	368	ASN	2.9
1	C	95	HIS	2.9
1	B	575	CYS	2.9
1	C	582	VAL	2.9
1	A	450	ALA	2.8
1	B	272	GLU	2.8
1	A	168	ASN	2.8
1	D	234	TYR	2.8
1	D	186	GLU	2.8
1	B	99	VAL	2.8
1	A	170	GLU	2.8
1	A	491	LEU	2.8
1	C	286	ALA	2.8
1	C	401	GLU	2.8
1	C	453	ASP	2.8
1	C	409	TYR	2.8
1	B	581	ASN	2.8
1	C	214	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	416	GLU	2.8
1	A	390	LEU	2.7
1	C	33	ALA	2.7
1	C	575	CYS	2.7
1	C	82	LEU	2.7
1	C	113	MET	2.7
1	D	377	ILE	2.7
1	A	272	GLU	2.7
1	A	186	GLU	2.7
1	B	491	LEU	2.6
1	B	186	GLU	2.6
1	D	583	GLN	2.6
1	C	239	ASP	2.6
1	A	296	PRO	2.6
1	A	399	ASP	2.6
1	A	515	ASP	2.6
1	B	102	ILE	2.6
1	A	486	GLU	2.6
1	C	215	LYS	2.6
1	D	54	GLN	2.6
1	A	441	PRO	2.6
1	A	83	LYS	2.6
1	A	473	LYS	2.6
1	B	98	GLY	2.5
1	C	59	CYS	2.5
1	D	74	PHE	2.5
1	D	91	TYR	2.5
1	A	222	ARG	2.5
1	C	428	ARG	2.5
1	B	290	GLU	2.5
1	B	352	LEU	2.5
1	B	198	PHE	2.5
1	B	426	PHE	2.5
1	A	508	LEU	2.5
1	D	316	LEU	2.5
1	D	328	LEU	2.5
1	A	116	VAL	2.5
1	C	295	VAL	2.5
1	A	482	THR	2.5
1	B	80	LEU	2.5
1	C	81	LEU	2.5
1	C	77	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	515	ASP	2.5
1	C	481	LEU	2.4
1	B	101	ASN	2.4
1	D	506	ALA	2.4
1	C	53	ASP	2.4
1	C	36	CYS	2.4
1	D	59	CYS	2.4
1	B	77	ARG	2.4
1	B	428	ARG	2.4
1	C	234	TYR	2.4
1	A	53	ASP	2.4
1	D	268	ASP	2.4
1	D	379	SER	2.4
1	B	493	ALA	2.4
1	C	170	GLU	2.4
1	B	341	ILE	2.4
1	C	186	GLU	2.4
1	A	148	TYR	2.4
1	D	409	TYR	2.4
1	A	93	LEU	2.3
1	A	373	TYR	2.3
1	D	500	VAL	2.3
1	B	51	GLY	2.3
1	B	252	LEU	2.3
1	D	473	LYS	2.3
1	A	157	ASP	2.3
1	B	485	LYS	2.3
1	C	491	LEU	2.3
1	C	158	ASP	2.3
1	A	562	ALA	2.3
1	B	221	THR	2.3
1	C	303	THR	2.3
1	B	107	PHE	2.3
1	B	363	PRO	2.3
1	B	75	LEU	2.3
1	D	329	PHE	2.3
1	B	52	PHE	2.2
1	B	73	GLU	2.2
1	B	506	ALA	2.2
1	B	515	ASP	2.2
1	C	515	ASP	2.2
1	D	165	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	107	PHE	2.2
1	D	113	MET	2.2
1	D	335	ILE	2.2
1	D	41	CYS	2.2
1	A	79	LYS	2.2
1	B	423	VAL	2.2
1	B	444	VAL	2.2
1	A	355	TYR	2.2
1	A	478	PHE	2.2
1	A	113	MET	2.2
1	A	214	HIS	2.2
1	C	416	GLU	2.2
1	A	398	GLU	2.1
1	B	234	TYR	2.1
1	D	352	LEU	2.1
1	A	98	GLY	2.1
1	C	258	GLY	2.1
1	B	106	PRO	2.1
1	A	535	MET	2.1
1	D	239	ASP	2.1
1	B	59	CYS	2.1
1	C	159	CYS	2.1
1	A	335	ILE	2.1
1	A	252	LEU	2.1
1	A	286	ALA	2.1
1	D	258	GLY	2.1
1	B	47	CYS	2.1
1	B	295	VAL	2.1
1	A	551	GLY	2.1
1	D	33	ALA	2.1
1	D	400	GLN	2.1
1	B	37	CYS	2.1
1	B	159	CYS	2.1
1	A	85	THR	2.1
1	D	148	TYR	2.1
1	A	56	LYS	2.1
1	A	41	CYS	2.0
1	C	395	PHE	2.0
1	C	508	LEU	2.0
1	D	390	LEU	2.0
1	B	91	TYR	2.0
1	D	214	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	233	ILE	2.0
1	B	500	VAL	2.0
1	D	256	VAL	2.0
1	A	514	PRO	2.0
1	A	287	VAL	2.0
1	B	294	LEU	2.0
1	C	316	LEU	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)

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^{th} 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^2)	Q<0.9
4	NAG	C	671	14/15	0.86	0.17	0.10	39,42,45,49	0
4	NAG	A	671	14/15	0.87	0.14	-0.75	40,43,46,50	0
4	NAG	D	671	14/15	0.92	0.12	-1.03	38,41,44,49	0
4	NAG	B	671	14/15	0.90	0.12	-2.11	40,42,46,50	0
4	NAG	D	673	14/15	0.58	0.52	-	62,64,64,64	0
4	NAG	D	672	14/15	0.78	0.31	-	53,56,57,60	0
4	NAG	B	672	14/15	0.78	0.39	-	54,58,59,61	0
4	NAG	A	673	14/15	0.49	0.56	-	63,64,65,65	0
4	NAG	A	672	14/15	0.68	0.27	-	53,55,58,60	0
4	NAG	B	673	14/15	0.59	0.70	-	63,65,66,66	0
4	NAG	C	673	14/15	0.49	0.59	-	62,63,64,64	0
4	NAG	C	672	14/15	0.60	0.38	-	53,56,57,60	0

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^{th} 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^2)	Q<0.9
3	NAG	B	661	14/15	0.70	0.40	5.12	48,51,53,53	0
3	NAG	C	681	14/15	0.72	0.44	3.33	48,51,53,53	0
5	BOG	D	8	20/20	0.63	0.28	2.99	63,63,63,63	0
3	NAG	A	681	14/15	0.82	0.32	2.93	44,47,48,48	0
5	BOG	A	7	20/20	0.59	0.35	2.48	64,65,66,66	0
5	BOG	A	703	20/20	0.68	0.27	1.97	58,58,60,60	0
5	BOG	B	6	20/20	0.78	0.25	1.27	72,72,72,72	0
3	NAG	D	681	14/15	0.79	0.25	0.84	46,49,50,50	0
3	NAG	B	681	14/15	0.82	0.37	0.69	48,50,51,51	0
5	BOG	C	5	20/20	0.85	0.18	0.37	60,60,62,62	0
2	HEM	A	619	43/43	0.88	0.19	0.10	44,45,49,50	0
2	HEM	C	619	43/43	0.88	0.18	-0.05	41,43,46,48	0
5	BOG	D	703	20/20	0.84	0.19	-0.06	51,51,55,55	0
2	HEM	D	619	43/43	0.90	0.17	-0.06	42,44,48,50	0
6	T1N	D	4	17/17	0.89	0.16	-0.28	40,41,41,42	0
6	T1N	B	1	17/17	0.92	0.15	-0.40	43,44,44,44	0
6	T1N	C	2	17/17	0.91	0.15	-0.45	41,41,42,43	0
6	T1N	A	3	17/17	0.91	0.15	-0.78	40,41,42,42	0
2	HEM	B	619	43/43	0.91	0.14	-1.24	46,47,49,50	0
3	NAG	A	661	14/15	0.77	0.44	-	47,50,51,51	0
3	NAG	C	661	14/15	0.80	0.38	-	47,50,51,51	0
3	NAG	D	661	14/15	0.76	0.43	-	47,50,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.