Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:03 AM GMT

PDB ID	:	3NTG
Title	:	Crystal structure of COX-2 with selective compound 23d-(R)
Authors	:	Wang, J.L.; Limburg, D.; Graneto, M.J.; Carter, J.C.; Talley, J.J.; Kiefer, J.R.
Deposited on	:	2010-07-04
Resolution	:	2.19 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:

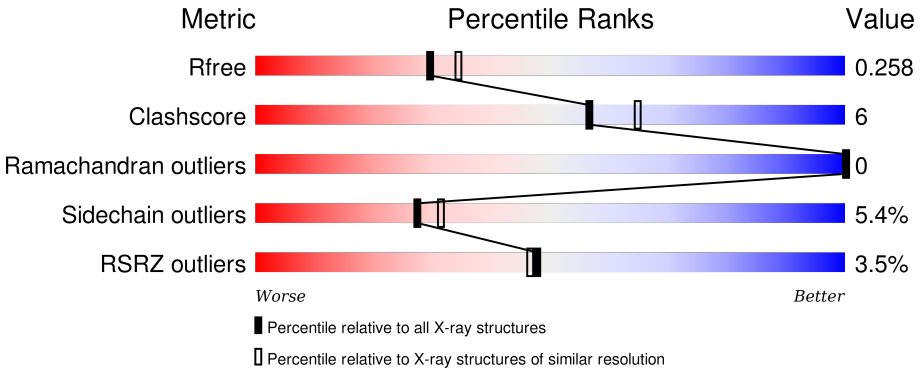
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	552	4% 86% 13%
1	B	552	3% 84% 14%
1	C	552	4% 85% 13%
1	D	552	3% 84% 14%

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
4	NAG	B	681	-	-	-	X
4	NAG	C	681	-	-	-	X

2 Entry composition

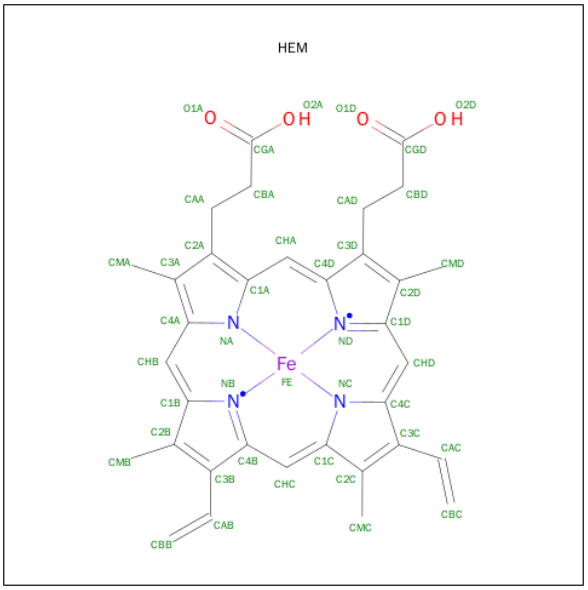
There are 7 unique types of molecules in this entry. The entry contains 19469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			4484	2890	752	817	25			
1	B	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	C	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	D	552	Total	C	N	O	S	0	1	0
			4482	2890	751	816	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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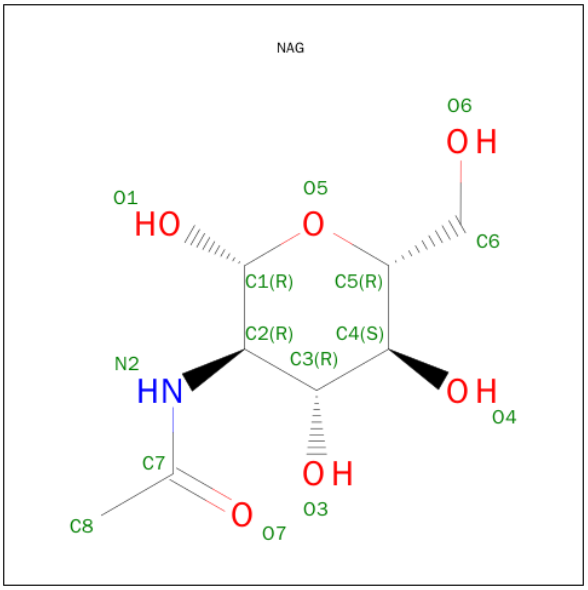
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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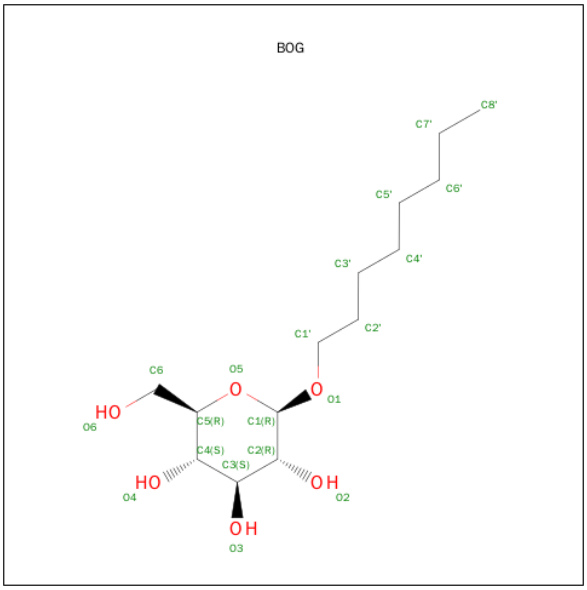
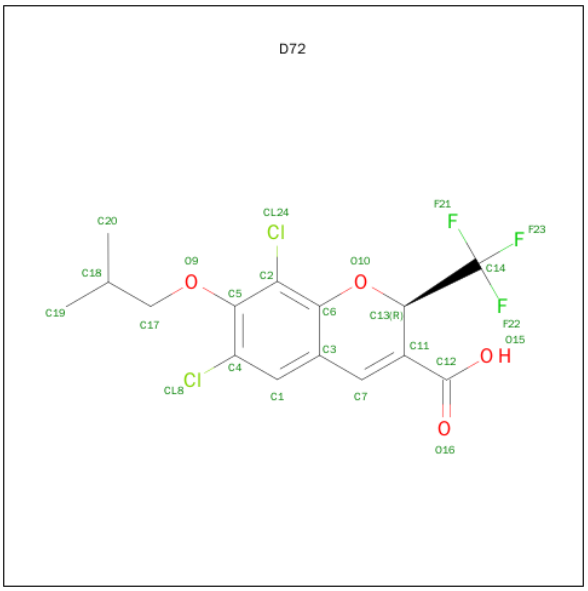
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is (2R)-6,8-DICHLORO-7-(2-METHYLPROPOXY)-2-(TRIFLUOROMETHYL)-2H-CHROMENE-3-CARBOXYLIC ACID (three-letter code: D72) (formula: $C_{15}H_{13}Cl_2F_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	F	O	0	0
			24	15	2	3	4		
6	B	1	Total	C	Cl	F	O	0	0
			24	15	2	3	4		
6	C	1	Total	C	Cl	F	O	0	0
			24	15	2	3	4		
6	D	1	Total	C	Cl	F	O	0	0
			24	15	2	3	4		

- Molecule 7 is water.

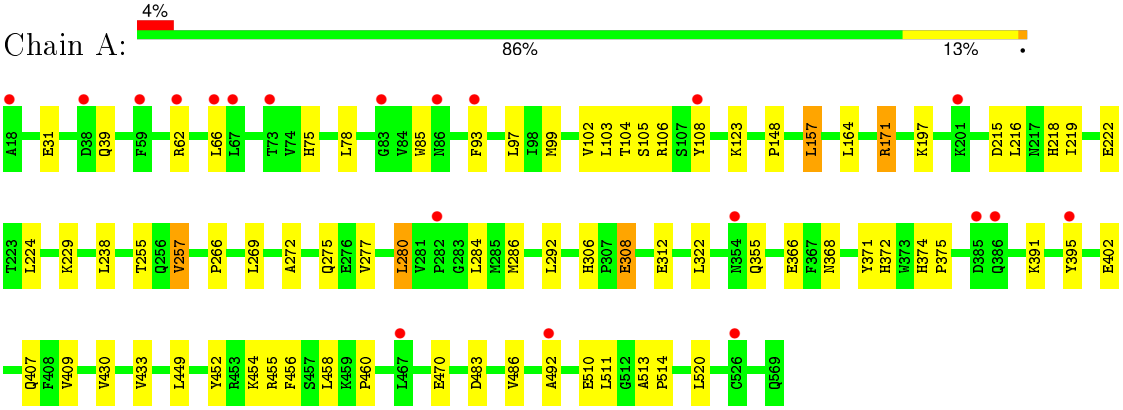
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	264	Total	O	0	0
			264	264		
7	B	296	Total	O	0	0
			296	296		
7	C	252	Total	O	0	0
			252	252		
7	D	265	Total	O	0	0
			265	265		

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.

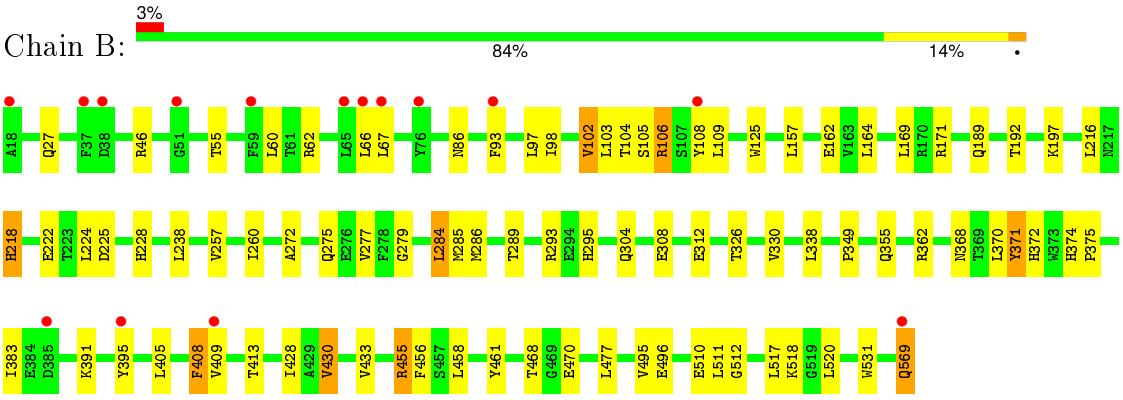
- Molecule 1: Prostaglandin G/H synthase 2

Chain A:



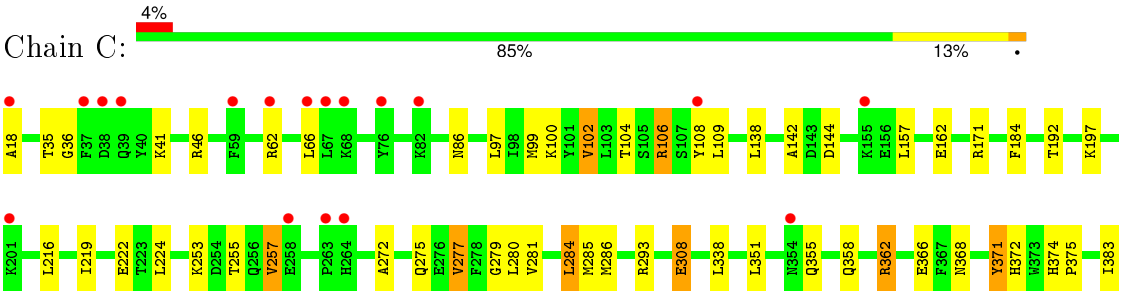
- Molecule 1: Prostaglandin G/H synthase 2

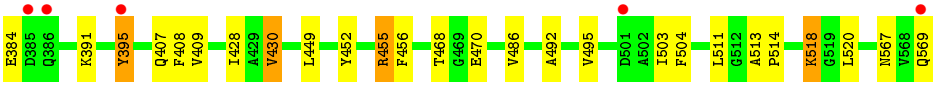
Chain B:



- Molecule 1: Prostaglandin G/H synthase 2

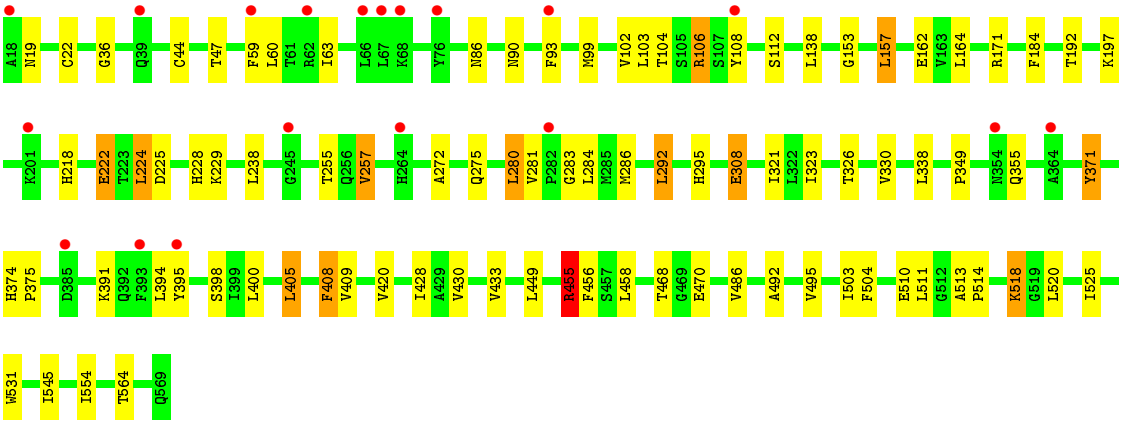
Chain C:





- Molecule 1: Prostaglandin G/H 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	180.27Å 134.27Å 122.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.19 – 2.19 19.93 – 2.19	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.19-2.19) 88.2 (19.93-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.255 0.213 , 0.258	Depositor DCC
R_{free} test set	13440 reflections (11.14%)	DCC
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	11 of 134086 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19469	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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 45.75 % 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 1.2634e-04.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: D72, HEM, 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	0.47	0/4611	0.62	2/6251 (0.0%)
1	B	0.47	0/4602	0.61	0/6239
1	C	0.43	0/4602	0.60	2/6239 (0.0%)
1	D	0.46	0/4609	0.61	2/6249 (0.0%)
All	All	0.46	0/18424	0.61	6/24978 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	455	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	362	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	362	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	D	455	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	455	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	171	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	4484	0	4381	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4475	0	4374	58	0
1	C	4475	0	4374	50	0
1	D	4482	0	4382	70	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	20	0	28	0	0
5	D	20	0	28	3	0
6	A	24	0	12	2	0
6	B	24	0	12	2	0
6	C	24	0	12	1	0
6	D	24	0	12	2	0
7	A	264	0	0	2	0
7	B	296	0	0	1	0
7	C	252	0	0	5	0
7	D	265	0	0	1	0
All	All	19469	0	17887	221	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 6.

All (221) 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:280:LEU:HD12	1:D:281:VAL:CG2	1.60	1.30
1:D:280:LEU:HD12	1:D:281:VAL:HG23	1.19	1.13
1:B:260:ILE:HD12	1:B:277:VAL:HG12	1.51	0.90
1:D:280:LEU:HD12	1:D:281:VAL:HG22	1.50	0.89
1:D:104:THR:HG21	1:D:355:GLN:HG2	1.57	0.86
1:D:280:LEU:CD1	1:D:281:VAL:CG2	2.50	0.85
1:B:456:PHE:CD2	1:B:511:LEU:HD22	2.18	0.78
1:C:104:THR:HG21	1:C:355:GLN:HG2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:CD1	1:D:281:VAL:HG22	2.14	0.76
1:A:104:THR:HG21	1:A:355:GLN:HG2	1.68	0.75
1:D:400:LEU:HD11	1:D:405:LEU:HD22	1.69	0.74
1:D:286:MET:HE2	1:D:409:VAL:HG22	1.70	0.73
1:A:216:LEU:HD13	1:A:219:ILE:HD12	1.73	0.70
1:B:109:LEU:O	1:B:455:ARG:NH2	2.25	0.70
1:D:280:LEU:CD1	1:D:281:VAL:HG23	2.10	0.70
1:C:109:LEU:O	1:C:455:ARG:NH2	2.25	0.70
1:D:456:PHE:CD2	1:D:511:LEU:HD22	2.27	0.69
1:C:104:THR:CG2	1:C:355:GLN:HG2	2.21	0.69
1:B:257:VAL:HG21	1:B:272:ALA:HB1	1.76	0.67
1:D:238:LEU:HD13	1:D:295:HIS:CD2	2.29	0.67
1:C:468:THR:HG22	1:C:495:VAL:CG1	2.25	0.66
1:B:197:LYS:NZ	1:B:222:GLU:HG2	2.10	0.66
1:C:308:GLU:HG3	1:D:36:GLY:C	2.16	0.66
1:B:257:VAL:CG2	1:B:272:ALA:HB1	2.26	0.65
1:A:197:LYS:HZ1	1:A:222:GLU:HG2	1.60	0.65
1:C:513:ALA:HB3	1:C:514:PRO:HD3	1.79	0.65
1:C:280:LEU:HD22	1:C:395:TYR:HD2	1.61	0.64
1:D:468:THR:HG22	1:D:495[A]:VAL:CG1	2.29	0.63
1:D:99:MET:O	1:D:102:VAL:HG22	1.99	0.61
1:C:279:GLY:HA2	1:C:285:MET:HE2	1.82	0.61
1:C:358:GLN:O	1:C:518:LYS:NZ	2.34	0.61
1:D:495[A]:VAL:O	1:D:495[A]:VAL:CG1	2.49	0.61
1:B:238:LEU:HD13	1:B:295:HIS:CD2	2.36	0.60
1:D:468:THR:HG22	1:D:495[A]:VAL:HG13	1.83	0.60
1:B:197:LYS:HZ1	1:B:222:GLU:CG	2.14	0.60
1:C:100:LYS:HE2	1:C:351:LEU:O	2.02	0.60
1:B:279:GLY:HA2	1:B:285:MET:HE2	1.85	0.59
1:C:216:LEU:HD13	1:C:219:ILE:HD12	1.85	0.59
1:B:197:LYS:HZ1	1:B:222:GLU:HG2	1.67	0.59
1:D:456:PHE:CG	1:D:511:LEU:HD22	2.38	0.58
1:A:266:PRO:HG2	1:A:269:LEU:HD12	1.86	0.58
1:C:449:LEU:HD22	1:C:492:ALA:CB	2.34	0.57
1:D:257:VAL:HG22	1:D:272:ALA:HB1	1.86	0.57
1:A:513:ALA:HB3	1:A:514:PRO:HD3	1.85	0.57
1:D:59:PHE:CZ	1:D:63:ILE:HD11	2.40	0.56
1:D:430:VAL:HG22	1:D:433:VAL:HB	1.87	0.56
1:B:286:MET:HE2	1:B:409:VAL:HG22	1.86	0.56
1:B:458:LEU:HD21	1:B:510:GLU:HG3	1.87	0.56
1:C:192:THR:HG21	1:C:371:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ILE:HD13	1:B:408:PHE:CE1	2.41	0.56
1:B:164:LEU:HD13	1:B:169:LEU:HG	1.88	0.56
1:A:286:MET:HE1	1:A:409:VAL:HG22	1.88	0.56
1:A:257:VAL:HG22	1:A:272:ALA:HB1	1.88	0.56
1:C:257:VAL:HG22	1:C:272:ALA:HB1	1.88	0.55
1:A:456:PHE:CG	1:A:511:LEU:HD22	2.41	0.55
1:A:255:THR:OG1	1:A:257:VAL:HG13	2.07	0.55
1:C:456:PHE:CD2	1:C:511:LEU:HD22	2.42	0.55
1:D:197:LYS:HZ1	1:D:222:GLU:HG2	1.72	0.55
1:C:279:GLY:HA2	1:C:285:MET:CE	2.37	0.55
1:D:280:LEU:O	1:D:280:LEU:HD13	2.06	0.55
1:B:60:LEU:HD12	1:B:60:LEU:O	2.08	0.54
1:A:197:LYS:HZ1	1:A:222:GLU:CG	2.19	0.54
6:A:701:D72:C17	6:A:701:D72:CL24	2.93	0.54
1:A:229:LYS:HB3	1:A:257:VAL:HG12	1.90	0.54
1:C:430:VAL:O	1:C:430:VAL:HG13	2.07	0.54
1:C:286:MET:HE2	1:C:409:VAL:HG22	1.91	0.53
1:C:468:THR:HG22	1:C:495:VAL:HG13	1.89	0.53
1:B:104:THR:HG21	1:B:355:GLN:CG	2.39	0.53
6:D:701:D72:CL24	6:D:701:D72:H17A	2.46	0.53
1:A:368:ASN:O	1:A:372:HIS:HD2	1.91	0.52
1:D:326:THR:O	1:D:330:VAL:HG23	2.10	0.52
1:D:102:VAL:O	1:D:106:ARG:HB2	2.09	0.52
1:C:197:LYS:NZ	1:C:222:GLU:HG2	2.24	0.52
1:B:46:ARG:NH1	7:B:4399:HOH:O	2.43	0.52
1:D:321:ILE:HA	1:D:545:ILE:HD11	1.92	0.52
1:B:468:THR:HG22	1:B:495:VAL:CG1	2.40	0.52
1:B:106:ARG:HG2	1:B:517:LEU:HD12	1.91	0.52
1:B:430:VAL:HG22	1:B:433:VAL:CG2	2.39	0.52
1:D:255:THR:OG1	1:D:257:VAL:HG13	2.10	0.52
1:D:257:VAL:CG2	1:D:272:ALA:HB1	2.40	0.51
1:A:449:LEU:HD22	1:A:492:ALA:CB	2.40	0.51
1:C:503:ILE:HG23	1:C:504:PHE:CG	2.46	0.51
1:B:430:VAL:HG13	1:B:430:VAL:O	2.10	0.51
1:D:374:HIS:N	1:D:375:PRO:CD	2.73	0.51
1:C:486:VAL:O	1:C:486:VAL:HG12	2.10	0.51
1:D:513:ALA:HB3	1:D:514:PRO:HD3	1.93	0.51
1:A:286:MET:CE	1:A:409:VAL:HG22	2.41	0.51
1:D:323:ILE:HG22	1:D:525:ILE:HD13	1.93	0.51
1:A:456:PHE:CD2	1:A:511:LEU:HD22	2.45	0.50
1:B:368:ASN:O	1:B:372:HIS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:HA2	1:B:285:MET:CE	2.41	0.50
1:A:75:HIS:HD2	7:A:5156:HOH:O	1.95	0.50
1:B:456:PHE:CG	1:B:511:LEU:HD22	2.47	0.49
1:C:18:ALA:HB3	1:C:144:ASP:OD2	2.12	0.49
1:B:430:VAL:HG22	1:B:433:VAL:HG21	1.94	0.49
1:D:495[A]:VAL:HG13	1:D:495[A]:VAL:O	2.12	0.49
1:C:100:LYS:NZ	7:C:4655:HOH:O	2.46	0.49
1:C:102:VAL:O	1:C:106:ARG:HB2	2.12	0.49
1:B:477:LEU:HD11	1:B:495:VAL:HG11	1.94	0.49
1:D:286:MET:HE1	1:D:409:VAL:N	2.27	0.49
1:A:75:HIS:HE1	7:A:5080:HOH:O	1.95	0.49
1:A:31:GLU:OE1	1:A:123:LYS:NZ	2.45	0.49
1:A:148:PRO:HG2	1:A:157:LEU:HD13	1.94	0.48
1:C:184:PHE:CZ	1:C:338:LEU:HD13	2.47	0.48
6:C:701:D72:CL24	6:C:701:D72:C17	2.98	0.48
1:D:197:LYS:NZ	1:D:222:GLU:HG2	2.28	0.48
1:A:99:MET:HA	1:A:102:VAL:HG22	1.95	0.48
1:D:280:LEU:HD13	1:D:394:LEU:HD22	1.96	0.48
1:D:458:LEU:HD11	1:D:510:GLU:HB2	1.96	0.48
1:A:366:GLU:HG2	1:A:452:TYR:CE1	2.47	0.48
1:A:197:LYS:NZ	1:A:222:GLU:HG2	2.28	0.48
1:C:286:MET:CE	1:C:409:VAL:HG22	2.44	0.48
1:B:62:ARG:O	1:B:66:LEU:HD13	2.14	0.48
1:B:458:LEU:HD11	1:B:510:GLU:HB2	1.96	0.47
1:D:184:PHE:CZ	1:D:338:LEU:HD13	2.49	0.47
1:D:428:ILE:HD11	5:D:703:BOG:H5'1	1.95	0.47
1:B:260:ILE:HD12	1:B:277:VAL:CG1	2.32	0.47
1:B:374:HIS:N	1:B:375:PRO:CD	2.77	0.47
1:A:374:HIS:N	1:A:375:PRO:CD	2.78	0.47
1:D:44:CYS:O	1:D:47:THR:HG23	2.14	0.47
1:D:238:LEU:HD23	1:D:292:LEU:HD23	1.96	0.47
1:A:483:ASP:HB3	1:A:486:VAL:HG23	1.96	0.47
1:B:97:LEU:O	1:B:97:LEU:HD23	2.14	0.47
1:B:197:LYS:NZ	1:B:222:GLU:CG	2.73	0.47
1:C:36:GLY:O	1:D:308:GLU:HG2	2.15	0.47
1:D:458:LEU:HD21	1:D:510:GLU:HG3	1.95	0.47
1:B:216:LEU:HD22	1:B:218:HIS:HE1	1.79	0.47
1:C:46:ARG:NH2	7:C:5014:HOH:O	2.46	0.46
1:C:62:ARG:O	1:C:66:LEU:HD13	2.14	0.46
1:B:104:THR:HG21	1:B:355:GLN:HG2	1.98	0.46
1:D:153:GLY:HA3	1:D:486:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:O	1:B:108:TYR:CD2	2.69	0.46
1:D:428:ILE:CD1	5:D:703:BOG:H8'3	2.45	0.46
1:B:286:MET:HE2	1:B:409:VAL:CG2	2.46	0.46
1:B:413:THR:HG22	1:B:569:GLN:HE22	1.81	0.46
1:D:138:LEU:HG	1:D:455:ARG:HG2	1.98	0.46
1:B:104:THR:HG21	1:B:355:GLN:HG3	1.98	0.45
1:B:349:PRO:HG2	1:B:531:TRP:CD2	2.51	0.45
1:C:138:LEU:HG	1:C:455:ARG:HG2	1.98	0.45
1:A:257:VAL:CG2	1:A:272:ALA:HB1	2.46	0.45
1:B:512:GLY:HA3	6:B:701:D72:H19B	1.97	0.45
1:D:224:LEU:HD22	1:D:228:HIS:NE2	2.32	0.45
1:B:286:MET:CE	1:B:409:VAL:CG2	2.95	0.45
1:D:349:PRO:HG2	1:D:531:TRP:CD2	2.52	0.45
1:B:286:MET:HG3	1:B:405:LEU:HD13	1.99	0.45
1:A:105:SER:O	1:A:108:TYR:CD2	2.70	0.45
1:C:97:LEU:C	1:C:97:LEU:HD23	2.36	0.45
1:C:293:ARG:NH2	7:C:4077:HOH:O	2.50	0.45
1:A:292:LEU:C	1:A:292:LEU:HD23	2.37	0.45
1:A:215:ASP:HB3	1:B:125:TRP:CZ2	2.52	0.45
1:C:384:GLU:OE1	1:C:407:GLN:HG2	2.17	0.45
1:A:458:LEU:HD21	1:A:510:GLU:HG3	1.98	0.45
1:D:104:THR:CG2	1:D:355:GLN:HG2	2.38	0.45
1:D:255:THR:CB	1:D:257:VAL:HG13	2.47	0.45
6:D:701:D72:CL24	6:D:701:D72:C17	3.02	0.45
1:B:370:LEU:HD12	1:B:370:LEU:C	2.37	0.45
1:B:98:ILE:O	1:B:102:VAL:HG13	2.17	0.45
1:D:449:LEU:HD22	1:D:492:ALA:CB	2.47	0.45
1:B:224:LEU:HD11	1:B:228:HIS:NE2	2.32	0.45
1:B:326:THR:O	1:B:330:VAL:HG23	2.16	0.44
1:C:253:LYS:NZ	7:C:5254:HOH:O	2.44	0.44
1:B:97:LEU:C	1:B:97:LEU:HD23	2.37	0.44
1:D:19:ASN:HB3	1:D:22:CYS:SG	2.58	0.44
1:A:430:VAL:HG22	1:A:433:VAL:HB	2.00	0.44
1:D:286:MET:CE	1:D:409:VAL:HG22	2.44	0.43
1:B:461:TYR:OH	1:B:496:GLU:OE2	2.33	0.43
1:D:554:ILE:HG12	1:D:564:THR:HG21	2.00	0.43
1:D:281:VAL:HG12	1:D:283:GLY:H	1.83	0.43
1:D:192:THR:HG21	1:D:371:TYR:CE2	2.53	0.43
1:B:192:THR:HG21	1:B:371:TYR:CE2	2.54	0.43
1:C:449:LEU:HD22	1:C:492:ALA:HB1	1.99	0.43
1:C:99:MET:HE3	1:C:102:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:MET:HA	1:D:102:VAL:HG22	2.00	0.43
1:A:216:LEU:HD11	1:A:322:LEU:HB3	2.01	0.43
1:A:449:LEU:HD22	1:A:492:ALA:HB1	2.00	0.43
1:D:112:SER:CB	1:D:518:LYS:HZ1	2.32	0.43
1:D:229:LYS:HB3	1:D:257:VAL:HG12	1.99	0.43
1:B:468:THR:HG22	1:B:495:VAL:HG13	1.99	0.43
1:A:62:ARG:O	1:A:66:LEU:HD13	2.19	0.43
1:C:277:VAL:HG13	1:C:277:VAL:O	2.18	0.43
2:B:601:HEM:HHC	2:B:601:HEM:HBB2	2.01	0.42
1:B:189:GLN:CG	1:B:284:LEU:HD11	2.49	0.42
1:B:286:MET:CE	1:B:409:VAL:HG23	2.50	0.42
1:C:486:VAL:O	1:C:486:VAL:CG1	2.67	0.42
1:C:197:LYS:HZ1	1:C:222:GLU:CG	2.32	0.42
1:B:164:LEU:HD11	1:B:169:LEU:HD21	2.01	0.42
1:A:277:VAL:O	1:A:280:LEU:HB2	2.19	0.42
1:D:286:MET:CE	1:D:409:VAL:CG2	2.97	0.42
1:D:157:LEU:HD12	7:D:4920:HOH:O	2.19	0.42
1:D:280:LEU:C	1:D:280:LEU:HD13	2.41	0.42
1:D:86:ASN:O	1:D:90:ASN:ND2	2.53	0.42
1:A:104:THR:HG21	1:A:355:GLN:CG	2.44	0.41
1:C:374:HIS:N	1:C:375:PRO:CD	2.83	0.41
1:D:430:VAL:O	1:D:430:VAL:HG22	2.20	0.41
1:B:27:GLN:HB2	1:B:55:THR:HG22	2.02	0.41
1:B:289:THR:HG22	1:B:293:ARG:HD3	2.01	0.41
1:A:78:LEU:HD13	1:A:85:TRP:CZ2	2.55	0.41
1:C:281:VAL:HB	1:C:284:LEU:HD22	2.03	0.41
1:C:216:LEU:HD13	1:C:219:ILE:CD1	2.51	0.41
1:C:368:ASN:O	1:C:372:HIS:HD2	2.04	0.41
1:C:142:ALA:HB1	7:C:4749:HOH:O	2.19	0.41
1:D:503:ILE:HG23	1:D:504:PHE:CG	2.56	0.41
6:B:701:D72:CL24	6:B:701:D72:C17	3.06	0.41
1:D:238:LEU:CD2	1:D:292:LEU:HD23	2.51	0.41
1:D:428:ILE:HD11	5:D:703:BOG:H8'3	2.01	0.41
1:C:255:THR:HB	1:C:257:VAL:HG13	2.03	0.41
1:C:366:GLU:HG2	1:C:452:TYR:CE1	2.56	0.41
1:D:375:PRO:HB2	1:D:420:VAL:HA	2.03	0.41
1:D:308:GLU:CD	1:D:308:GLU:H	2.25	0.41
1:A:306:HIS:HA	1:A:308:GLU:OE2	2.21	0.41
1:D:255:THR:HB	1:D:257:VAL:HG13	2.03	0.40
1:B:569:GLN:HG2	1:B:569:GLN:O	2.20	0.40
1:A:454:LYS:HD2	1:A:460:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:MET:O	1:D:102:VAL:CG2	2.68	0.40
1:C:35:THR:HG21	1:C:41:LYS:HB2	2.03	0.40
1:C:257:VAL:CG2	1:C:272:ALA:HB1	2.50	0.40
6:A:701:D72:H17	6:A:701:D72:CL24	2.59	0.40
1:C:383:ILE:HD13	1:C:408:PHE:CE1	2.56	0.40
1:D:286:MET:CE	1:D:408:PHE:HB3	2.51	0.40
1:B:413:THR:CG2	1:B:569:GLN:HE22	2.35	0.40
1:A:407:GLN:HA	1:A:407:GLN:NE2	2.37	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	551/552 (100%)	537 (98%)	14 (2%)	0	100	100
1	B	550/552 (100%)	535 (97%)	15 (3%)	0	100	100
1	C	550/552 (100%)	535 (97%)	15 (3%)	0	100	100
1	D	551/552 (100%)	536 (97%)	15 (3%)	0	100	100
All	All	2202/2208 (100%)	2143 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	494/493 (100%)	471 (95%)	23 (5%)	32 39
1	B	493/493 (100%)	464 (94%)	29 (6%)	24 27
1	C	493/493 (100%)	468 (95%)	25 (5%)	29 34
1	D	494/493 (100%)	465 (94%)	29 (6%)	24 27
All	All	1974/1972 (100%)	1868 (95%)	106 (5%)	27 31

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	93	PHE
1	A	97	LEU
1	A	103	LEU
1	A	106	ARG
1	A	157	LEU
1	A	164	LEU
1	A	171	ARG
1	A	218	HIS
1	A	224	LEU
1	A	238	LEU
1	A	257	VAL
1	A	275	GLN
1	A	280	LEU
1	A	284	LEU
1	A	308	GLU
1	A	312	GLU
1	A	371	TYR
1	A	391	LYS
1	A	395	TYR
1	A	402	GLU
1	A	470	GLU
1	A	520	LEU
1	B	67	LEU
1	B	86	ASN
1	B	93	PHE
1	B	102	VAL
1	B	103	LEU
1	B	106	ARG
1	B	157	LEU
1	B	162	GLU
1	B	171	ARG
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	225	ASP
1	B	275	GLN
1	B	284	LEU
1	B	304	GLN
1	B	308	GLU
1	B	312	GLU
1	B	338	LEU
1	B	362	ARG
1	B	371	TYR
1	B	391	LYS
1	B	395	TYR
1	B	408	PHE
1	B	428	ILE
1	B	430	VAL
1	B	455	ARG
1	B	470	GLU
1	B	518	LYS
1	B	520	LEU
1	B	569	GLN
1	C	86	ASN
1	C	102	VAL
1	C	106	ARG
1	C	108	TYR
1	C	157	LEU
1	C	162	GLU
1	C	171	ARG
1	C	224	LEU
1	C	257	VAL
1	C	275	GLN
1	C	277	VAL
1	C	284	LEU
1	C	308	GLU
1	C	362	ARG
1	C	371	TYR
1	C	391	LYS
1	C	395	TYR
1	C	428	ILE
1	C	430	VAL
1	C	455	ARG
1	C	470	GLU
1	C	518	LYS
1	C	520	LEU

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Mol	Chain	Res	Type
1	C	567	ASN
1	C	569	GLN
1	D	60	LEU
1	D	93	PHE
1	D	103	LEU
1	D	106	ARG
1	D	108	TYR
1	D	157	LEU
1	D	162	GLU
1	D	164	LEU
1	D	171	ARG
1	D	218	HIS
1	D	222	GLU
1	D	224	LEU
1	D	225	ASP
1	D	257	VAL
1	D	275	GLN
1	D	280	LEU
1	D	284	LEU
1	D	292	LEU
1	D	308	GLU
1	D	371	TYR
1	D	391	LYS
1	D	395	TYR
1	D	398	SER
1	D	405	LEU
1	D	408	PHE
1	D	455	ARG
1	D	470	GLU
1	D	518	LYS
1	D	520	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	304	GLN
1	A	342	HIS
1	A	372	HIS
1	A	407	GLN
1	B	86	ASN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	569	GLN
1	C	86	ASN
1	C	567	ASN
1	D	86	ASN
1	D	567	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

8 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	$\#\|Z\|>2$
3	NAG	A	671	1,3	14,14,15	0.52	0	15,19,21	1.43	3 (20%)
3	NAG	A	672	3	14,14,15	0.47	0	15,19,21	1.27	2 (13%)
3	NAG	B	671	1,3	14,14,15	0.61	0	15,19,21	1.56	1 (6%)
3	NAG	B	672	3	14,14,15	0.41	0	15,19,21	1.10	1 (6%)
3	NAG	C	671	1,3	14,14,15	0.65	0	15,19,21	1.26	1 (6%)
3	NAG	C	672	3	14,14,15	0.47	0	15,19,21	1.42	2 (13%)
3	NAG	D	671	1,3	14,14,15	0.61	0	15,19,21	1.57	1 (6%)
3	NAG	D	672	3	14,14,15	0.50	0	15,19,21	1.17	2 (13%)

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
3	NAG	A	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	NAG	B	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	672	3	-	0/6/23/26	0/1/1/1
3	NAG	C	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	672	3	-	0/6/23/26	0/1/1/1
3	NAG	D	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	672	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	672	NAG	C4-C3-C2	-2.84	106.81	111.23
3	A	672	NAG	C4-C3-C2	-2.79	106.90	111.23
3	D	672	NAG	C4-C3-C2	-2.72	107.00	111.23
3	A	671	NAG	C2-N2-C7	-2.27	120.13	123.04
3	A	671	NAG	O4-C4-C3	-2.06	105.69	110.34
3	B	672	NAG	O5-C5-C6	2.52	112.80	107.35
3	D	672	NAG	C3-C2-N2	2.55	116.67	110.56
3	A	672	NAG	C3-C2-N2	2.66	116.93	110.56
3	C	672	NAG	C1-O5-C5	3.59	116.80	112.25
3	C	671	NAG	C1-O5-C5	4.27	117.67	112.25
3	A	671	NAG	C1-O5-C5	4.41	117.84	112.25
3	D	671	NAG	C1-O5-C5	5.05	118.66	112.25
3	B	671	NAG	C1-O5-C5	5.35	119.04	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

14 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	601	1,7	30,50,50	2.13	6 (20%)	24,82,82	2.55	12 (50%)
4	NAG	A	681	1	14,14,15	0.51	0	15,19,21	0.95	0
6	D72	A	701	-	21,25,25	0.88	0	30,38,38	1.49	6 (20%)
5	BOG	A	703	-	20,20,20	0.42	0	25,25,25	1.04	1 (4%)
2	HEM	B	601	1,7	30,50,50	2.24	7 (23%)	24,82,82	2.41	12 (50%)
4	NAG	B	681	1	14,14,15	0.68	0	15,19,21	1.26	2 (13%)
6	D72	B	701	-	21,25,25	0.82	0	30,38,38	1.52	6 (20%)
2	HEM	C	601	1,7	30,50,50	2.15	5 (16%)	24,82,82	2.35	12 (50%)
4	NAG	C	681	1	14,14,15	0.58	0	15,19,21	1.17	2 (13%)
6	D72	C	701	-	21,25,25	0.78	0	30,38,38	1.44	3 (10%)
2	HEM	D	601	1	30,50,50	2.03	6 (20%)	24,82,82	2.48	14 (58%)
4	NAG	D	681	1	14,14,15	0.56	0	15,19,21	1.04	0
6	D72	D	701	-	21,25,25	0.79	0	30,38,38	1.35	2 (6%)
5	BOG	D	703	-	20,20,20	0.43	0	25,25,25	0.77	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	601	1,7	-	0/10/54/54	0/0/8/8
4	NAG	A	681	1	-	0/6/23/26	0/1/1/1
6	D72	A	701	-	-	0/11/27/27	0/2/2/2
5	BOG	A	703	-	-	0/11/31/31	0/1/1/1
2	HEM	B	601	1,7	-	0/10/54/54	0/0/8/8
4	NAG	B	681	1	-	0/6/23/26	0/1/1/1
6	D72	B	701	-	-	0/11/27/27	0/2/2/2
2	HEM	C	601	1,7	-	0/10/54/54	0/0/8/8
4	NAG	C	681	1	-	0/6/23/26	0/1/1/1
6	D72	C	701	-	-	0/11/27/27	0/2/2/2
2	HEM	D	601	1	-	0/10/54/54	0/0/8/8
4	NAG	D	681	1	-	0/6/23/26	0/1/1/1
6	D72	D	701	-	-	0/11/27/27	0/2/2/2
5	BOG	D	703	-	-	0/11/31/31	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-C4B	-6.95	1.45	1.51
2	A	601	HEM	C3B-C4B	-6.93	1.45	1.51
2	C	601	HEM	C3B-C4B	-6.66	1.45	1.51
2	B	601	HEM	C3D-C4D	-6.14	1.43	1.51
2	D	601	HEM	C3B-C4B	-6.08	1.46	1.51
2	C	601	HEM	C3D-C4D	-6.06	1.43	1.51
2	A	601	HEM	C3D-C4D	-5.66	1.44	1.51
2	D	601	HEM	C3D-C4D	-5.46	1.44	1.51
2	A	601	HEM	C2C-C1C	-4.19	1.44	1.52
2	B	601	HEM	C2C-C1C	-4.11	1.44	1.52
2	D	601	HEM	C2C-C1C	-3.63	1.45	1.52
2	C	601	HEM	C2C-C1C	-3.60	1.45	1.52
2	C	601	HEM	C2D-C1D	-2.52	1.43	1.51
2	D	601	HEM	C2B-C1B	-2.46	1.43	1.51
2	B	601	HEM	C2D-C1D	-2.36	1.44	1.51
2	A	601	HEM	C2B-C1B	-2.35	1.44	1.51
2	A	601	HEM	C2D-C1D	-2.34	1.44	1.51
2	B	601	HEM	C2B-C1B	-2.23	1.44	1.51
2	D	601	HEM	C2D-C1D	-2.16	1.44	1.51
2	A	601	HEM	C1C-NC	2.01	1.38	1.36
2	D	601	HEM	FE-NC	2.04	2.03	1.95
2	C	601	HEM	C1C-NC	2.22	1.38	1.36
2	B	601	HEM	C1C-NC	2.34	1.38	1.36
2	B	601	HEM	FE-NC	2.36	2.05	1.95

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	HEM	CBA-CAA-C2A	-4.69	104.12	112.53
2	A	601	HEM	C3B-CAB-CBB	-3.73	118.74	124.46
6	A	701	D72	O9-C5-C4	-3.66	116.81	121.19
2	B	601	HEM	CBD-CAD-C3D	-3.41	103.63	113.55
6	B	701	D72	O10-C6-C2	-3.34	114.04	118.20
2	A	601	HEM	C3C-CAC-CBC	-3.22	119.52	124.46
6	C	701	D72	O9-C5-C4	-3.19	117.37	121.19
2	C	601	HEM	CBD-CAD-C3D	-3.17	104.33	113.55
6	C	701	D72	C3-C7-C11	-3.13	115.80	121.50
2	C	601	HEM	C3B-CAB-CBB	-3.10	119.70	124.46
2	A	601	HEM	CBA-CAA-C2A	-3.05	107.07	112.53
2	A	601	HEM	CBD-CAD-C3D	-3.03	104.75	113.55
2	B	601	HEM	C3C-CAC-CBC	-2.97	119.89	124.46
6	B	701	D72	C3-C7-C11	-2.85	116.30	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	701	D72	C3-C7-C11	-2.82	116.36	121.50
2	D	601	HEM	C3C-CAC-CBC	-2.81	120.14	124.46
2	C	601	HEM	C3C-CAC-CBC	-2.79	120.18	124.46
6	B	701	D72	O9-C5-C4	-2.57	118.11	121.19
6	A	701	D72	C3-C7-C11	-2.55	116.85	121.50
2	B	601	HEM	CBA-CAA-C2A	-2.47	108.10	112.53
2	B	601	HEM	C3B-C4B-NB	-2.44	106.96	111.63
2	D	601	HEM	CMA-C3A-C4A	-2.35	124.48	128.36
2	B	601	HEM	C3B-CAB-CBB	-2.30	120.92	124.46
2	C	601	HEM	C3B-C4B-NB	-2.26	107.31	111.63
2	D	601	HEM	C3B-C4B-NB	-2.22	107.38	111.63
2	D	601	HEM	CAA-C2A-C1A	-2.22	124.60	127.01
2	D	601	HEM	C3B-CAB-CBB	-2.20	121.08	124.46
6	B	701	D72	C17-O9-C5	-2.07	106.12	113.88
2	A	601	HEM	CMA-C3A-C4A	-2.06	124.95	128.36
2	D	601	HEM	CBD-CAD-C3D	-2.03	107.64	113.55
2	C	601	HEM	C2C-C1C-CHC	2.00	126.73	123.68
2	D	601	HEM	C2D-C3D-C4D	2.03	104.94	101.50
4	C	681	NAG	C3-C4-C5	2.05	113.76	110.20
2	A	601	HEM	C2D-C3D-C4D	2.06	104.99	101.50
6	A	701	D72	C1-C4-CL8	2.22	121.92	118.50
2	D	601	HEM	CMD-C2D-C3D	2.39	124.91	114.35
2	B	601	HEM	C2D-C3D-C4D	2.53	105.79	101.50
6	B	701	D72	C5-C2-CL24	2.59	123.25	118.87
4	B	681	NAG	C3-C4-C5	2.69	114.88	110.20
2	C	601	HEM	C2D-C3D-C4D	2.69	106.06	101.50
2	A	601	HEM	CMD-C2D-C3D	2.76	126.54	114.35
2	A	601	HEM	C3B-C4B-CHC	2.80	127.10	123.16
6	A	701	D72	F22-C14-C13	2.84	115.64	111.66
2	B	601	HEM	CMD-C2D-C3D	2.92	127.28	114.35
2	C	601	HEM	CMC-C2C-C3C	2.93	123.84	116.53
4	C	681	NAG	C4-C3-C2	2.93	115.78	111.23
2	D	601	HEM	C3B-C4B-CHC	2.96	127.33	123.16
6	A	701	D72	O9-C5-C2	3.01	124.67	120.66
4	B	681	NAG	C4-C3-C2	3.08	116.02	111.23
2	C	601	HEM	CMD-C2D-C3D	3.10	128.07	114.35
2	C	601	HEM	C3B-C4B-CHC	3.16	127.61	123.16
2	B	601	HEM	C3B-C4B-CHC	3.17	127.63	123.16
2	B	601	HEM	CMC-C2C-C3C	3.21	124.55	116.53
6	A	701	D72	C3-C6-C2	3.27	120.82	116.05
6	C	701	D72	C3-C6-C2	3.34	120.92	116.05
2	C	601	HEM	CMB-C2B-C3B	3.41	125.03	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	703	BOG	O1-C1-C2	3.44	112.38	108.04
2	D	601	HEM	CMC-C2C-C3C	3.45	125.16	116.53
6	B	701	D72	C3-C6-C2	3.57	121.25	116.05
2	B	601	HEM	CMB-C2B-C3B	3.63	125.61	116.53
2	D	601	HEM	CMB-C2B-C3B	3.72	125.81	116.53
6	D	701	D72	C3-C6-C2	3.77	121.56	116.05
2	C	601	HEM	CAD-C3D-C4D	3.81	125.91	112.47
2	B	601	HEM	CAD-C3D-C4D	3.83	125.98	112.47
2	A	601	HEM	CMC-C2C-C3C	3.96	126.42	116.53
2	A	601	HEM	CMB-C2B-C3B	4.05	126.65	116.53
2	A	601	HEM	CAD-C3D-C4D	4.11	126.95	112.47
2	D	601	HEM	CAD-C3D-C4D	4.42	128.05	112.47
2	D	601	HEM	CAD-C3D-C2D	4.79	126.98	113.22
2	C	601	HEM	CAD-C3D-C2D	5.13	127.97	113.22
2	A	601	HEM	CAD-C3D-C2D	5.14	128.00	113.22
2	B	601	HEM	CAD-C3D-C2D	5.20	128.16	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	D72	2	0
2	B	601	HEM	1	0
6	B	701	D72	2	0
6	C	701	D72	1	0
6	D	701	D72	2	0
5	D	703	BOG	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^{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	552/552 (100%)	0.17	20 (3%)	46	45	29, 41, 56, 73	0
1	B	552/552 (100%)	0.09	15 (2%)	58	57	30, 41, 57, 74	0
1	C	552/552 (100%)	0.22	23 (4%)	40	39	32, 45, 64, 79	0
1	D	552/552 (100%)	0.24	19 (3%)	49	47	30, 44, 62, 76	0
All	All	2208/2208 (100%)	0.18	77 (3%)	48	46	29, 43, 61, 79	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	569	GLN	7.7
1	D	108	TYR	7.3
1	B	569	GLN	7.3
1	A	108	TYR	7.1
1	D	18	ALA	6.4
1	C	59	PHE	5.6
1	C	67	LEU	5.5
1	B	108	TYR	5.0
1	C	108	TYR	4.5
1	B	67	LEU	4.5
1	B	18	ALA	4.3
1	A	395	TYR	3.9
1	A	18	ALA	3.9
1	C	39	GLN	3.8
1	D	67	LEU	3.7
1	A	59	PHE	3.6
1	A	67	LEU	3.6
1	D	66	LEU	3.6
1	C	395	TYR	3.6
1	D	395	TYR	3.4
1	B	395	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	385	ASP	3.2
1	D	93	PHE	3.1
1	B	385	ASP	3.1
1	D	62	ARG	3.1
1	C	38	ASP	3.0
1	C	68	LYS	3.0
1	A	201	LYS	3.0
1	A	354	ASN	3.0
1	B	93	PHE	3.0
1	C	18	ALA	3.0
1	D	354	ASN	3.0
1	A	38	ASP	3.0
1	B	59	PHE	2.9
1	C	201	LYS	2.9
1	A	66	LEU	2.8
1	C	385	ASP	2.8
1	D	59	PHE	2.8
1	B	65	LEU	2.7
1	B	51	GLY	2.7
1	C	258	GLU	2.7
1	C	264	HIS	2.6
1	B	38	ASP	2.6
1	D	264	HIS	2.6
1	A	385	ASP	2.6
1	D	201	LYS	2.6
1	A	282	PRO	2.6
1	A	73	THR	2.6
1	B	66	LEU	2.6
1	A	83	GLY	2.5
1	D	282	PRO	2.4
1	C	386	GLN	2.4
1	C	501	ASP	2.4
1	A	93	PHE	2.4
1	D	76	TYR	2.3
1	A	62	ARG	2.3
1	C	354	ASN	2.3
1	D	364	ALA	2.2
1	C	155	LYS	2.2
1	A	386	GLN	2.2
1	C	62	ARG	2.2
1	A	526	CYS	2.2
1	B	37	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	2.2
1	A	86	ASN	2.2
1	B	76	TYR	2.2
1	D	39	GLN	2.1
1	C	82	LYS	2.1
1	D	68	LYS	2.1
1	D	393	PHE	2.1
1	B	409	VAL	2.1
1	C	37	PHE	2.1
1	A	467	LEU	2.1
1	D	245	GLY	2.1
1	C	263	PRO	2.0
1	C	76	TYR	2.0
1	C	66	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
3	NAG	B	671	14/15	0.91	0.13	0.19	32,35,37,42	0
3	NAG	C	671	14/15	0.94	0.12	0.03	35,39,41,44	0
3	NAG	D	671	14/15	0.92	0.10	-0.65	36,40,41,44	0
3	NAG	A	671	14/15	0.95	0.10	-0.65	34,36,39,43	0
3	NAG	A	672	14/15	0.78	0.24	-	47,51,52,53	0
3	NAG	D	672	14/15	0.84	0.20	-	47,50,50,52	0
3	NAG	C	672	14/15	0.86	0.29	-	48,51,52,54	0
3	NAG	B	672	14/15	0.85	0.32	-	45,48,50,50	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
4	NAG	C	681	14/15	0.83	0.37	3.12	53,56,58,58	0
4	NAG	B	681	14/15	0.83	0.29	2.25	50,53,54,54	0
4	NAG	D	681	14/15	0.83	0.27	1.51	47,49,50,50	0
4	NAG	A	681	14/15	0.80	0.23	1.00	46,49,50,50	0
2	HEM	B	601	43/43	0.95	0.13	0.27	28,33,47,51	0
2	HEM	C	601	43/43	0.95	0.12	-0.02	29,34,48,53	0
5	BOG	D	703	20/20	0.92	0.12	-0.07	43,48,57,58	0
6	D72	C	701	24/24	0.94	0.12	-0.25	42,44,47,48	0
2	HEM	D	601	43/43	0.95	0.12	-0.35	31,33,40,46	0
2	HEM	A	601	43/43	0.96	0.11	-0.36	29,32,43,49	0
6	D72	A	701	24/24	0.94	0.11	-0.46	38,42,43,45	0
6	D72	D	701	24/24	0.93	0.11	-0.47	41,43,47,48	0
5	BOG	A	703	20/20	0.95	0.12	-0.66	35,40,49,49	0
6	D72	B	701	24/24	0.95	0.10	-0.77	38,40,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.