Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:01 AM GMT

PDB ID	:	3KK6
Title	:	Crystal Structure of Cyclooxygenase-1 in complex with celecoxib
Authors	:	Sidhu, R.S.
Deposited on	:	2009-11-04
Resolution	:	2.75 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:

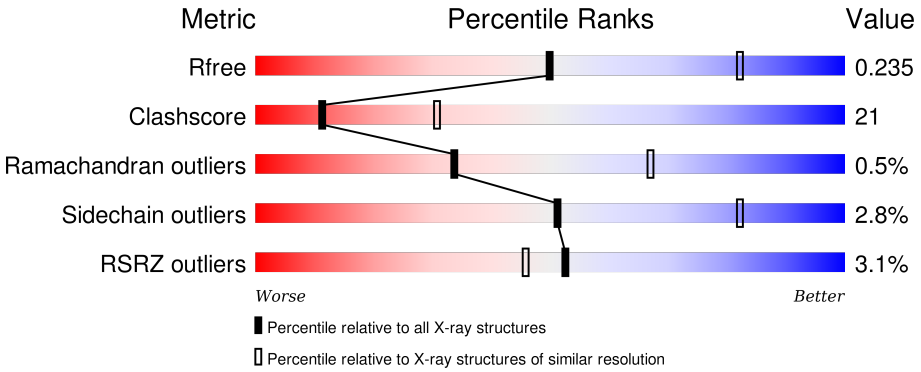
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	553	3% 71% 27%
1	B	553	4% 68% 29%

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	671	-	-	X	-
3	MAN	A	673	-	-	X	-
3	BMA	A	674	-	-	X	-
3	MAN	A	675	-	-	X	-
4	NAG	B	1681	-	-	X	-
5	CEL	A	701	-	-	X	-
5	CEL	B	1701	-	-	-	X
6	BOG	B	1751	-	-	X	-
6	BOG	B	1752	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18050 atoms, of which 8678 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.

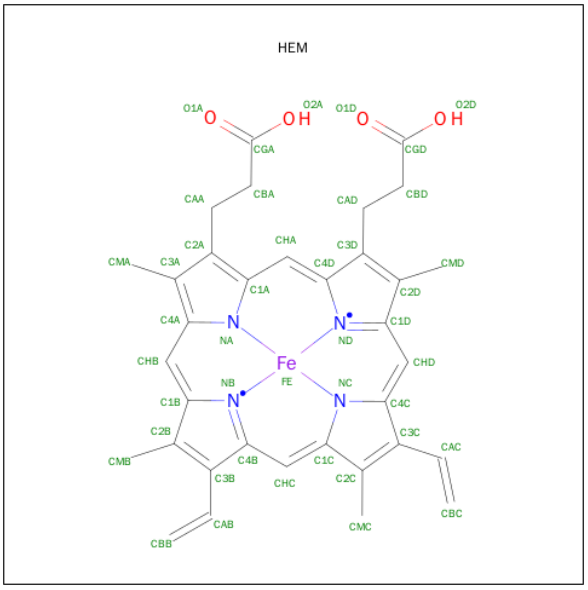
- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	H	N	O	S	4120	1	0
			8497	2840	4120	731	778	28			
1	B	553	Total	C	H	N	O	S	4219	12	0
			8670	2899	4206	742	795	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	SEE REMARK 999	UNP P05979
B	92	LEU	MET	SEE REMARK 999	UNP P05979

- 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	H	N	O	30	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Fe	H	N	O	30	0
			73	34	1	30	4	4		

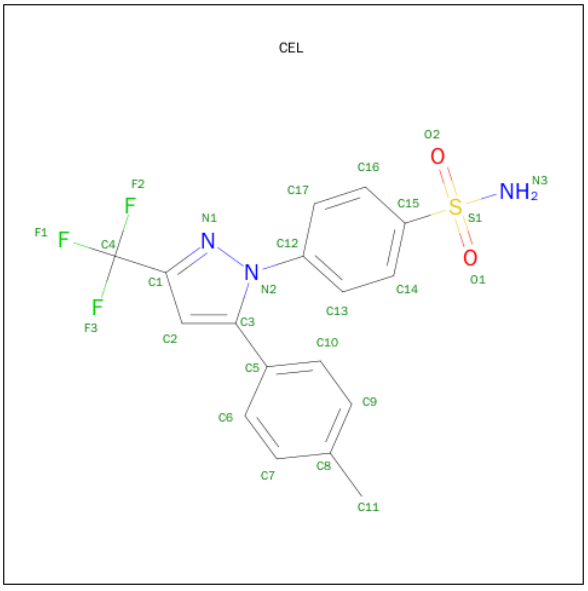
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	5	Total	C	H	N	O	33	0
			94	34	33	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	2	Total	C	H	N	O	25	0
			53	16	25	2	10		
4	B	2	Total	C	H	N	O	25	0
			53	16	25	2	10		
4	B	2	Total	C	H	N	O	25	0
			53	16	25	2	10		

- Molecule 5 is 4-[5-(4-METHYLPHENYL)-3-(TRIFLUOROMETHYL)-1H-PYRAZOL-1-YL]BENZENESULFONAMIDE (three-letter code: CEL) (formula: $C_{17}H_{14}F_3N_3O_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	S	14	0
			40	17	3	14	3	2	1		

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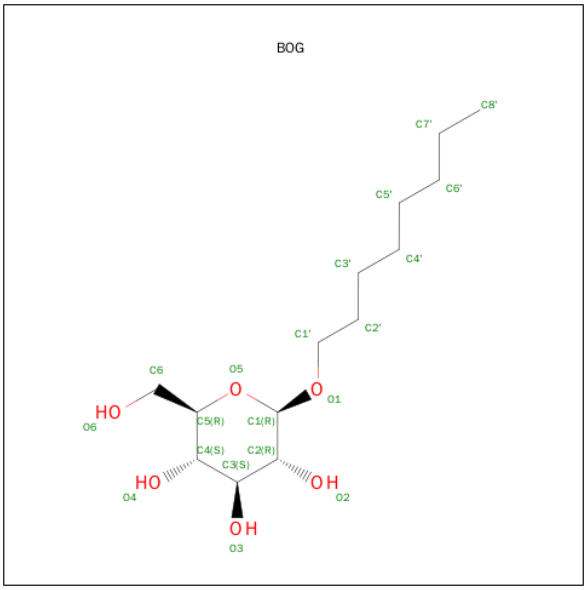
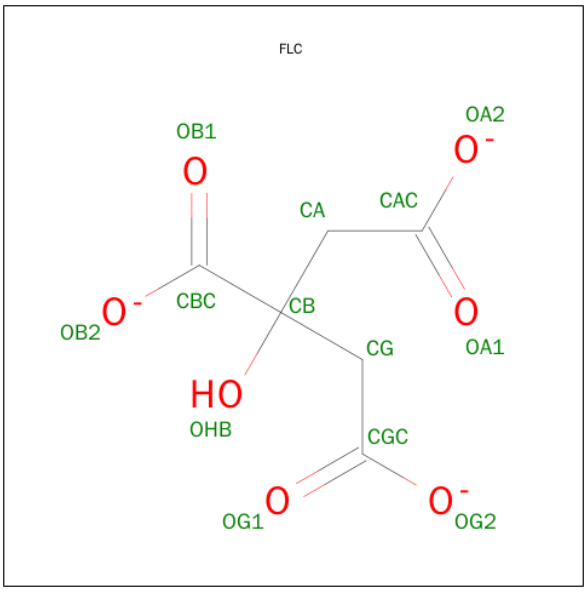
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	F	H	N	O	S	14	0
			40	17	3	14	3	2	1		

- Molecule 6 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	30	0
			47	14	27	6		
6	A	1	Total	C	H	O	28	0
			48	14	28	6		
6	B	1	Total	C	H	O	28	0
			48	14	28	6		
6	B	1	Total	C	H	O	28	0
			48	14	28	6		

- Molecule 7 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	5	0
			18	6	5	7		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	4	Total	C	H	N	O	40	0
			90	28	40	2	20		

- Molecule 9 is water.

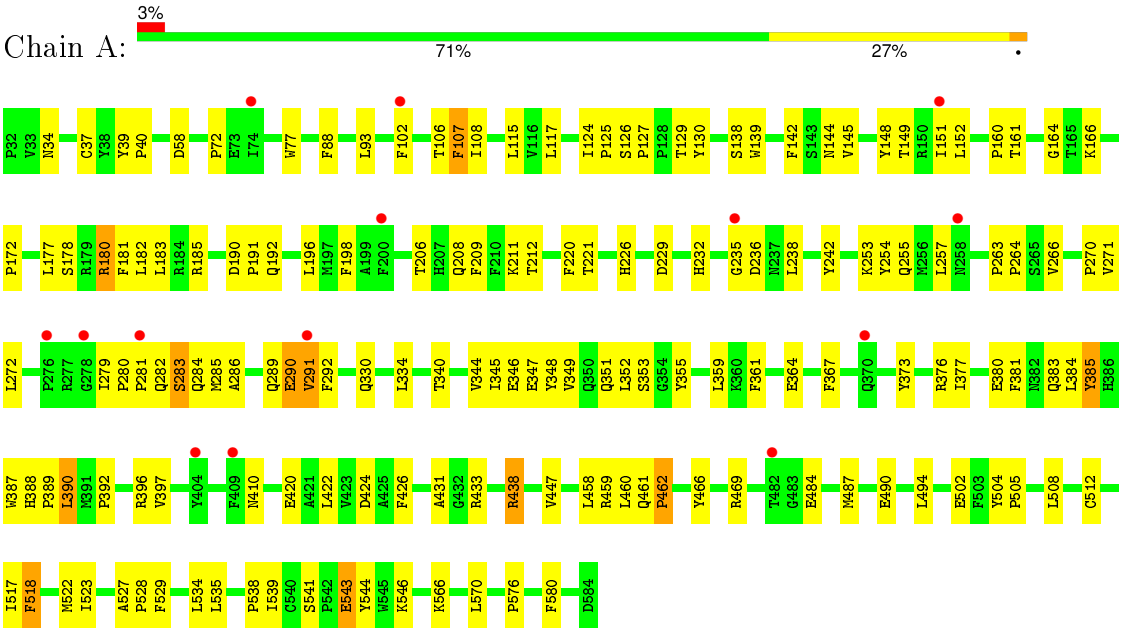
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	55	Total	O	0	0
			55	55		
9	B	50	Total	O	0	0
			50	50		

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.

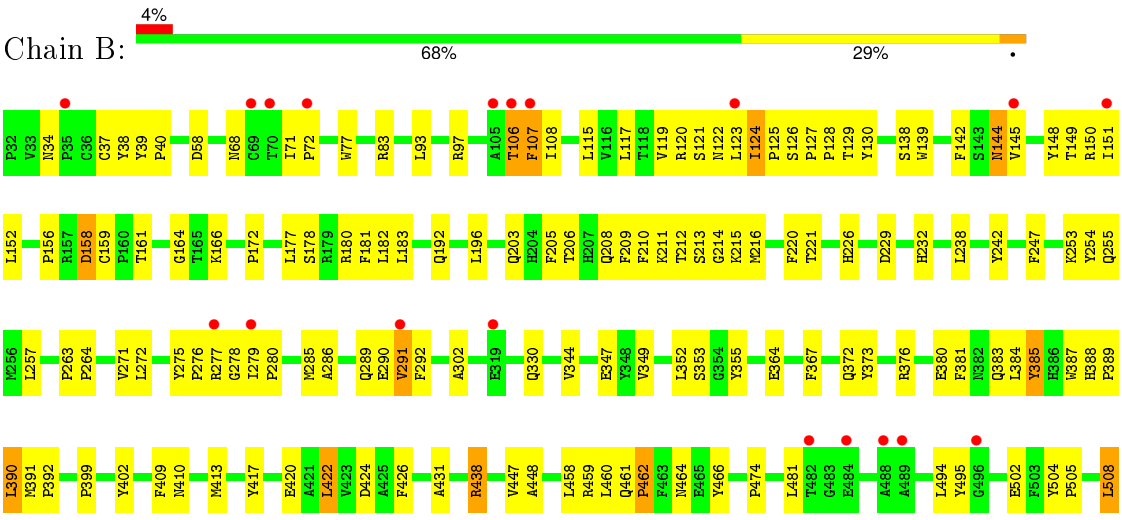
- Molecule 1: Prostaglandin G/H synthase 1

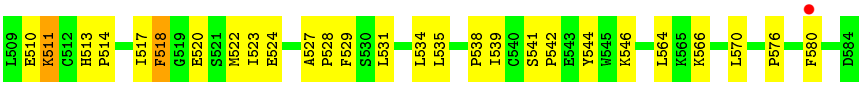
Chain A:



- Molecule 1: Prostaglandin G/H synthase 1

Chain B:




L509
E510
K511
C512
H513
P514
I517
F518
G519
E520
S521
M522
I523
E524
A527
P528
F529
S530
I531
L534
L535
P538
I539
C540
S541
P542
E543
Y544
W545
K546
L564
K565
K566
L570
P576
F580
D584

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	181.03Å 181.03Å 102.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.41 – 2.75 46.58 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.41-2.75) 97.4 (46.58-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.207 , 0.242 0.203 , 0.235	Depositor DCC
R_{free} test set	1959 reflections (4.20%)	DCC
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.9	EDS
Estimated twinning fraction	0.501 for h,-h-k,-l 0.489 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.501 for h,-h-k,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 49651 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18050	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: BMA, NAG, CEL, NDG, HEM, FLC, BOG, MAN

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	0.45	2/4517 (0.0%)	0.55	6/6155 (0.1%)
1	B	0.44	0/4610	0.56	7/6287 (0.1%)
All	All	0.44	2/9127 (0.0%)	0.55	13/12442 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543[A]	GLU	N-CA	5.09	1.56	1.46
1	A	543[B]	GLU	N-CA	5.09	1.56	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	459	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	A	459	ARG	NE-CZ-NH1	-12.53	114.03	120.30
1	B	459	ARG	NE-CZ-NH1	12.42	126.51	120.30
1	A	459	ARG	NE-CZ-NH2	12.25	126.43	120.30
1	B	180	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	180	ARG	NE-CZ-NH1	-11.86	114.37	120.30
1	A	180	ARG	NE-CZ-NH2	11.67	126.14	120.30
1	B	180	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	B	97	ARG	NE-CZ-NH1	6.31	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	459	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	459	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	180	ARG	CD-NE-CZ	5.32	131.04	123.60
1	B	180	ARG	CD-NE-CZ	5.17	130.84	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124[B]	ILE	Peptide

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	4377	4120	4173	144	0
1	B	4464	4206	4244	200	1
2	A	43	30	30	7	0
2	B	43	30	30	10	0
3	A	61	33	52	28	0
4	A	28	25	25	2	1
4	B	56	50	50	18	0
5	A	26	14	14	9	0
5	B	26	14	14	8	0
6	A	40	55	56	4	0
6	B	40	56	55	13	0
7	A	13	5	4	0	0
8	B	50	40	43	13	0
9	A	55	0	0	3	0
9	B	50	0	0	3	0
All	All	9372	8678	8790	372	1

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 21.

All (372) 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:144:ASN:HD21	3:A:671:NAG:C1	0.96	1.55
1:A:144:ASN:ND2	3:A:671:NAG:C1	1.80	1.36
3:A:674:BMA:O4	3:A:675:MAN:C2	1.81	1.28
3:A:674:BMA:O4	3:A:675:MAN:H2	1.22	1.26
1:B:349:VAL:O	1:B:353:SER:OG	1.53	1.26
1:B:125[B]:PRO:HB2	1:B:372:GLN:CB	1.67	1.24
1:B:125[B]:PRO:CB	1:B:372:GLN:HB2	1.71	1.19
1:B:410:ASN:OD1	4:B:1681:NAG:C1	1.92	1.18
1:B:216:MET:HG2	8:B:1672:NAG:H83	1.27	1.17
3:A:674:BMA:O4	3:A:675:MAN:C5	1.92	1.16
3:A:674:BMA:O4	3:A:675:MAN:H5	1.45	1.15
1:B:144:ASN:OD1	8:B:1671:NAG:C1	1.97	1.11
1:A:433:ARG:HH21	1:A:512:CYS:HB2	1.12	1.10
1:A:543[B]:GLU:HB2	1:B:126[B]:SER:HB2	1.29	1.09
3:A:674:BMA:O4	3:A:675:MAN:C1	2.01	1.09
1:B:83:ARG:NH2	6:B:1751:BOG:O3	1.86	1.08
1:A:543[A]:GLU:OE2	1:B:125[A]:PRO:HA	1.56	1.06
1:B:216:MET:HG2	8:B:1672:NAG:C8	1.87	1.05
8:B:1673:MAN:O6	8:B:1674:BMA:H62	1.52	1.04
1:B:83:ARG:HH21	6:B:1751:BOG:C3	1.72	1.02
1:A:433:ARG:NH2	1:A:512:CYS:HB2	1.78	0.97
1:B:276:PRO:HD2	1:B:279:ILE:HD11	1.47	0.96
3:A:674:BMA:O4	3:A:675:MAN:O5	1.86	0.92
1:B:83:ARG:NH2	6:B:1751:BOG:C3	2.32	0.91
1:B:83:ARG:HH21	6:B:1751:BOG:H3	1.34	0.91
3:A:674:BMA:HO4	3:A:675:MAN:H2	0.93	0.90
3:A:674:BMA:HO4	3:A:675:MAN:C2	1.77	0.89
1:B:68:ASN:HD21	4:B:1661:NAG:C1	1.87	0.88
1:B:290:GLU:O	1:B:291:VAL:HG23	1.74	0.88
3:A:674:BMA:C4	3:A:675:MAN:H2	1.98	0.86
1:B:120[A]:ARG:HD3	6:B:1751:BOG:H62	1.59	0.85
1:B:277:ARG:CB	1:B:278:GLY:CA	2.56	0.84
1:B:277:ARG:CB	1:B:278:GLY:HA3	2.08	0.84
1:B:216:MET:CG	8:B:1672:NAG:H83	2.08	0.83
1:A:433:ARG:HH21	1:A:512:CYS:CB	1.93	0.81
3:A:673:MAN:O6	3:A:674:BMA:C1	2.29	0.80
1:B:410:ASN:CG	4:B:1681:NAG:C1	2.49	0.80
1:B:290:GLU:O	1:B:291:VAL:CG2	2.31	0.78
1:B:124[B]:ILE:HG22	1:B:124[B]:ILE:O	1.83	0.78
1:B:83:ARG:NH2	6:B:1751:BOG:H3	1.94	0.78
8:B:1673:MAN:O6	8:B:1674:BMA:C6	2.29	0.78
1:B:238:LEU:HD21	1:B:242:TYR:CE2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PRO:HD3	1:A:433:ARG:HD2	1.65	0.77
3:A:672:NAG:C1	3:A:672:NAG:O7	2.30	0.77
1:B:410:ASN:ND2	4:B:1681:NAG:C1	2.48	0.77
1:B:410:ASN:HD21	4:B:1681:NAG:C1	1.97	0.77
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.69	0.75
3:A:671:NAG:HO6	3:A:672:NAG:C1	2.01	0.74
1:B:120[B]:ARG:HD3	6:B:1751:BOG:H62	1.70	0.73
3:A:673:MAN:C6	3:A:674:BMA:C1	2.66	0.73
1:A:191:PRO:CD	1:A:433:ARG:HD2	2.19	0.72
1:A:410:ASN:HD21	4:A:681:NAG:C1	2.03	0.71
1:A:190:ASP:OD2	1:A:192:GLN:HB2	1.89	0.71
3:A:674:BMA:HO4	3:A:675:MAN:H5	1.51	0.71
1:B:277:ARG:CB	1:B:279:ILE:HG13	2.20	0.71
3:A:671:NAG:O6	3:A:672:NAG:C1	2.40	0.70
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.74	0.70
1:A:282:GLN:O	1:A:283:SER:CB	2.39	0.69
1:A:144:ASN:CG	3:A:671:NAG:C1	2.61	0.69
1:A:352:LEU:O	5:A:701:CEL:N3	2.23	0.69
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.73	0.69
1:B:279:ILE:HG22	1:B:280:PRO:N	2.09	0.68
1:B:115:LEU:O	1:B:119:VAL:HB	1.94	0.68
1:A:102:PHE:O	1:A:106:THR:HG23	1.95	0.67
1:B:68:ASN:ND2	4:B:1661:NAG:C1	2.57	0.67
1:B:144:ASN:CG	8:B:1671:NAG:C1	2.62	0.67
2:B:601:HEM:HMB1	2:B:601:HEM:HBB2	1.77	0.67
1:A:388:HIS:N	1:A:389:PRO:CD	2.58	0.67
1:A:282:GLN:O	1:A:283:SER:HB3	1.95	0.66
1:A:279:ILE:HG23	1:A:281:PRO:HD3	1.78	0.66
1:B:417:TYR:HB3	1:B:422:LEU:HD13	1.79	0.65
1:A:39:TYR:N	1:A:40:PRO:HD3	2.11	0.65
1:A:352:LEU:O	5:A:701:CEL:H14C	1.96	0.65
1:B:518:PHE:CE1	5:B:1701:CEL:O1	2.49	0.65
9:A:596:HOH:O	1:B:542:PRO:HD2	1.95	0.65
1:A:144:ASN:ND2	3:A:671:NAG:O5	2.16	0.64
3:A:673:MAN:HO6	3:A:674:BMA:C1	2.07	0.64
1:A:543[B]:GLU:HB2	1:B:126[B]:SER:CB	2.17	0.64
1:B:276:PRO:HD2	1:B:279:ILE:CD1	2.26	0.64
1:B:448:ALA:HA	9:B:616:HOH:O	1.96	0.64
1:B:388:HIS:N	1:B:389:PRO:CD	2.58	0.64
1:B:523:ILE:HD11	5:B:1701:CEL:S1	2.38	0.64
1:A:352:LEU:O	5:A:701:CEL:C14	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG23	1:B:152:LEU:N	2.12	0.62
1:A:517:ILE:HG22	5:A:701:CEL:N3	2.14	0.62
1:A:115:LEU:HD23	6:A:751:BOG:H4'2	1.82	0.62
1:B:352:LEU:HG	5:B:1701:CEL:H14C	1.82	0.61
1:A:192:GLN:OE1	5:A:701:CEL:N3	2.33	0.61
1:A:238:LEU:HD21	1:A:242:TYR:CE2	2.36	0.60
1:B:524:GLU:OE2	6:B:1751:BOG:H2	2.00	0.60
1:B:124[B]:ILE:CG2	1:B:124[B]:ILE:O	2.50	0.60
1:A:129:THR:HG22	9:A:597:HOH:O	2.01	0.60
1:B:211:LYS:O	1:B:212:THR:C	2.38	0.60
1:B:148:TYR:CZ	1:B:221:THR:HB	2.37	0.59
1:A:539:ILE:HA	1:A:544:TYR:HB3	1.85	0.59
1:B:344:VAL:O	1:B:349:VAL:HG23	2.01	0.59
3:A:673:MAN:O6	3:A:674:BMA:C2	2.51	0.59
1:B:216:MET:CG	8:B:1672:NAG:C8	2.73	0.59
1:B:68:ASN:HD21	4:B:1661:NAG:C2	2.16	0.59
1:A:172:PRO:HG3	1:A:494:LEU:HB3	1.84	0.59
1:B:151:ILE:CG2	1:B:152:LEU:N	2.66	0.59
3:A:674:BMA:H3	3:A:675:MAN:O2	2.02	0.58
1:B:277:ARG:CB	1:B:278:GLY:C	2.72	0.58
1:A:538:PRO:HG3	1:B:142:PHE:CZ	2.39	0.58
1:B:539:ILE:HA	1:B:544:TYR:HB3	1.84	0.58
1:B:391:MET:HE3	2:B:601:HEM:HHC	1.84	0.58
1:B:144:ASN:ND2	8:B:1671:NAG:C1	2.66	0.58
1:B:172:PRO:HG3	1:B:494:LEU:HB3	1.85	0.58
1:B:39:TYR:N	1:B:40:PRO:HD3	2.19	0.58
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.86	0.58
1:B:216:MET:HG2	8:B:1672:NAG:H82	1.84	0.57
1:B:144:ASN:HD21	8:B:1671:NAG:C1	2.17	0.57
2:B:601:HEM:HHA	2:B:601:HEM:HBA2	1.85	0.57
1:A:138:SER:HB2	1:B:330:GLN:CG	2.34	0.57
1:B:208:GLN:HG3	1:B:209:PHE:CD2	2.39	0.57
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.85	0.57
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.41	0.56
1:A:352:LEU:HG	5:A:701:CEL:H14C	1.88	0.56
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.41	0.56
1:A:196:LEU:HD21	1:A:392:PRO:HG3	1.88	0.56
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.41	0.56
1:A:420:GLU:HB2	1:A:576:PRO:HG3	1.88	0.56
1:B:289:GLN:HG2	1:B:292:PHE:CE1	2.41	0.56
1:B:120[A]:ARG:CZ	6:B:1751:BOG:H1'2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HG	1:B:535:LEU:CD1	2.36	0.55
1:A:126:SER:HA	1:A:127:PRO:C	2.26	0.55
1:A:290:GLU:O	1:A:291:VAL:HG23	2.05	0.55
1:A:387:TRP:HB3	1:A:390:LEU:HD12	1.88	0.55
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.88	0.55
1:B:402:TYR:HE1	4:B:1682:NDG:O	1.90	0.55
1:A:138:SER:HB2	1:B:330:GLN:HG2	1.88	0.55
1:B:387:TRP:HB3	1:B:390:LEU:HD12	1.88	0.55
1:B:517:ILE:HG23	1:B:518:PHE:CD2	2.42	0.55
1:B:196:LEU:HD21	1:B:392:PRO:HG3	1.88	0.54
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.41	0.54
1:A:518:PHE:CG	1:A:522:MET:HG2	2.41	0.54
1:B:120[A]:ARG:HD3	6:B:1751:BOG:C6	2.35	0.54
1:A:117:LEU:HG	1:A:535:LEU:CD1	2.37	0.54
1:B:178:SER:HA	1:B:182:LEU:HB2	1.90	0.54
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.88	0.54
1:B:420:GLU:HB2	1:B:576:PRO:HG3	1.88	0.54
1:B:349:VAL:O	1:B:353:SER:CB	2.54	0.54
1:B:417:TYR:CB	1:B:422:LEU:HD13	2.38	0.54
1:A:93:LEU:HD13	1:A:355:TYR:CE2	2.43	0.54
1:B:518:PHE:CD1	5:B:1701:CEL:O1	2.61	0.53
1:A:178:SER:HA	1:A:182:LEU:HB2	1.90	0.53
1:A:364:GLU:HA	1:A:367:PHE:CD1	2.44	0.53
1:B:390:LEU:HD23	1:B:431:ALA:HB1	1.91	0.53
1:B:161:THR:HG22	1:B:164:GLY:C	2.29	0.53
1:B:122[B]:ASN:CG	1:B:123[B]:LEU:H	2.12	0.53
1:B:290:GLU:C	1:B:291:VAL:CG2	2.75	0.53
1:A:518:PHE:CD1	1:A:522:MET:HB3	2.44	0.53
1:A:211:LYS:O	1:A:212:THR:C	2.46	0.52
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.43	0.52
1:A:263:PRO:HB2	1:A:285:MET:HB3	1.91	0.52
1:A:88:PHE:HB2	6:A:754:BOG:H2'2	1.90	0.52
1:A:330:GLN:CG	1:B:138:SER:HB2	2.39	0.52
1:A:344:VAL:O	1:A:349:VAL:HG23	2.10	0.52
1:B:144:ASN:OD1	8:B:1671:NAG:O5	2.25	0.52
1:A:390:LEU:HD23	1:A:431:ALA:HB1	1.91	0.52
1:A:161:THR:HG22	1:A:164:GLY:C	2.29	0.52
1:B:364:GLU:HA	1:B:367:PHE:CD1	2.44	0.52
1:B:502:GLU:HB2	1:B:505:PRO:HG2	1.92	0.51
1:A:373:TYR:CZ	1:A:541:SER:HA	2.46	0.51
1:B:495:TYR:OH	1:B:502:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PRO:HB2	1:B:285:MET:HB3	1.92	0.51
1:B:120[B]:ARG:CZ	6:B:1751:BOG:H1'2	2.40	0.51
1:B:279:ILE:CG2	1:B:280:PRO:N	2.73	0.51
1:B:278:GLY:O	1:B:279:ILE:HB	2.10	0.51
1:B:373:TYR:CZ	1:B:541:SER:HA	2.46	0.51
4:B:1662:NDG:C3	4:B:1662:NDG:O7	2.57	0.51
1:B:210:PHE:HB3	2:B:601:HEM:HBD1	1.92	0.51
1:B:125[B]:PRO:HB3	9:B:614:HOH:O	2.09	0.50
1:A:212:THR:HA	1:A:220:PHE:O	2.11	0.50
1:A:353:SER:HA	5:A:701:CEL:C14	2.41	0.50
1:B:253:LYS:C	1:B:264:PRO:HG3	2.32	0.50
1:A:212:THR:OG1	2:A:601:HEM:O1D	2.27	0.50
1:B:513:HIS:HB3	1:B:514:PRO:CD	2.42	0.50
1:B:355:TYR:OH	5:B:1701:CEL:H17C	2.12	0.50
1:A:353:SER:HA	5:A:701:CEL:C15	2.41	0.50
1:B:93:LEU:HB3	1:B:355:TYR:CD1	2.47	0.50
1:B:523:ILE:HD11	5:B:1701:CEL:O1	2.12	0.49
4:B:1661:NAG:O3	4:B:1662:NDG:O	2.29	0.49
1:B:192:GLN:HE22	5:B:1701:CEL:HN31	1.61	0.49
1:A:253:LYS:C	1:A:264:PRO:HG3	2.32	0.49
1:B:203:GLN:HB2	2:B:601:HEM:HMC3	1.95	0.49
3:A:671:NAG:O4	3:A:671:NAG:O6	2.30	0.49
1:A:546:LYS:HB3	1:B:58:ASP:OD2	2.13	0.49
1:B:238:LEU:CD2	1:B:242:TYR:CE2	2.92	0.49
1:B:129[A]:THR:HG23	1:B:130[A]:TYR:N	2.28	0.49
1:B:504:TYR:CZ	1:B:508:LEU:HD21	2.48	0.49
1:A:334:LEU:HD11	1:B:138:SER:HA	1.94	0.49
1:A:255:GLN:HG2	1:A:257:LEU:HD13	1.95	0.49
1:A:198:PHE:HB2	1:A:580:PHE:HD1	1.78	0.49
1:A:384:LEU:C	1:A:384:LEU:HD12	2.33	0.49
1:A:145:VAL:HG13	1:A:226:HIS:CD2	2.48	0.49
1:A:142:PHE:CZ	1:B:538:PRO:HG3	2.48	0.49
1:A:124:ILE:HD11	1:A:529:PHE:HA	1.94	0.48
1:B:384:LEU:C	1:B:384:LEU:HD12	2.33	0.48
3:A:673:MAN:O6	3:A:674:BMA:O2	2.30	0.48
1:A:388:HIS:N	1:A:389:PRO:HD2	2.29	0.48
1:A:125:PRO:HD3	1:A:151:ILE:CD1	2.42	0.48
4:B:1662:NDG:O3	4:B:1662:NDG:O7	2.30	0.48
1:A:232:HIS:HA	1:A:289:GLN:HB2	1.96	0.48
1:B:156:PRO:C	1:B:158:ASP:H	2.16	0.48
1:B:255:GLN:HG2	1:B:257:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LYS:HA	1:B:570:LEU:HD13	1.95	0.48
1:B:125[B]:PRO:CG	1:B:372:GLN:H	2.26	0.48
1:B:564:LEU:HD22	1:B:580:PHE:CZ	2.48	0.48
1:B:123[B]:LEU:O	1:B:124[B]:ILE:C	2.51	0.48
1:B:424:ASP:HB2	1:B:576:PRO:HB3	1.96	0.48
1:B:255:GLN:HB2	1:B:264:PRO:HA	1.96	0.48
1:A:255:GLN:HB2	1:A:264:PRO:HA	1.96	0.48
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.44	0.47
1:B:145:VAL:HG13	1:B:226:HIS:CD2	2.48	0.47
1:A:192:GLN:NE2	1:A:351:GLN:O	2.47	0.47
1:A:490:GLU:O	1:A:494:LEU:HD13	2.14	0.47
1:B:71:ILE:O	1:B:71:ILE:HG23	2.14	0.47
1:B:124[A]:ILE:CD1	1:B:529:PHE:HA	2.43	0.47
2:A:601:HEM:HHA	2:A:601:HEM:HBA2	1.95	0.47
1:A:566:LYS:HA	1:A:570:LEU:HD13	1.95	0.47
1:B:413:MET:HE3	4:B:1681:NAG:H61	1.96	0.47
1:A:349:VAL:HG12	1:A:349:VAL:O	2.15	0.47
1:B:347:GLU:HB3	1:B:580:PHE:HE2	1.78	0.47
2:B:601:HEM:CMB	2:B:601:HEM:HBB2	2.42	0.47
1:A:523:ILE:HD11	5:A:701:CEL:O2	2.15	0.47
1:B:290:GLU:C	1:B:291:VAL:HG22	2.34	0.47
1:B:447:VAL:HG13	2:B:601:HEM:HBA1	1.96	0.47
1:A:424:ASP:HB2	1:A:576:PRO:HB3	1.96	0.47
1:B:232:HIS:HA	1:B:289:GLN:HB2	1.97	0.47
1:B:121[B]:SER:O	1:B:122[B]:ASN:HB3	2.15	0.47
6:A:754:BOG:O5	6:A:754:BOG:C2'	2.60	0.46
3:A:673:MAN:H62	3:A:674:BMA:C1	2.44	0.46
1:B:123[B]:LEU:C	1:B:125[B]:PRO:HD2	2.35	0.46
1:B:123[B]:LEU:O	1:B:124[B]:ILE:HB	2.15	0.46
1:B:120[B]:ARG:HG3	1:B:531:LEU:HD12	1.97	0.46
1:B:388:HIS:N	1:B:389:PRO:HD2	2.29	0.46
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.55	0.46
4:B:1681:NAG:O4	4:B:1682:NDG:O7	2.33	0.46
1:B:276:PRO:HG2	1:B:409:PHE:HB3	1.97	0.46
2:B:601:HEM:CBA	2:B:601:HEM:HHA	2.46	0.46
1:B:279:ILE:HG22	1:B:280:PRO:O	2.15	0.46
1:A:279:ILE:O	1:A:281:PRO:CD	2.63	0.46
1:A:484:GLU:OE1	1:A:487:MET:HB2	2.16	0.46
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.55	0.46
1:B:216:MET:HA	8:B:1672:NAG:C8	2.46	0.46
1:B:510:GLU:OE2	1:B:520[A]:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG23	1:B:152:LEU:HG	1.98	0.46
4:B:1661:NAG:HO3	4:B:1662:NDG:C1	2.29	0.46
1:B:390:LEU:HD23	1:B:431:ALA:CB	2.46	0.46
1:A:149:THR:HB	1:A:376:ARG:HG2	1.98	0.46
1:B:125[B]:PRO:HB2	1:B:372:GLN:HB2	0.75	0.45
1:A:390:LEU:HD23	1:A:431:ALA:CB	2.46	0.45
1:A:151:ILE:HD11	1:A:469:ARG:NH2	2.31	0.45
1:B:242:TYR:CD1	1:B:247:PHE:HZ	2.34	0.45
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.44	0.45
1:B:125[B]:PRO:HG3	1:B:372:GLN:H	1.81	0.45
1:A:279:ILE:O	1:A:281:PRO:HD2	2.16	0.45
1:B:149:THR:HB	1:B:376:ARG:HG2	1.98	0.45
1:A:148:TYR:CZ	1:A:221:THR:HB	2.51	0.45
1:A:39:TYR:N	1:A:40:PRO:CD	2.79	0.45
1:A:172:PRO:HB2	1:A:177:LEU:HD11	1.98	0.45
1:B:172:PRO:HB2	1:B:177:LEU:HD11	1.99	0.45
1:B:123[B]:LEU:HD22	1:B:123[B]:LEU:N	2.32	0.45
1:A:543[A]:GLU:OE2	1:B:125[A]:PRO:CA	2.46	0.45
1:B:242:TYR:CD1	1:B:247:PHE:CZ	3.04	0.45
1:A:517:ILE:HG23	1:A:518:PHE:CD2	2.51	0.45
1:A:284:GLN:O	1:A:284:GLN:CG	2.65	0.45
1:A:290:GLU:O	1:A:291:VAL:CG2	2.65	0.44
4:B:1681:NAG:O3	4:B:1682:NDG:O6	2.33	0.44
1:B:129[A]:THR:HG23	1:B:130[A]:TYR:CD2	2.52	0.44
1:A:208:GLN:HG3	1:A:209:PHE:CD2	2.52	0.44
1:B:539:ILE:HA	1:B:544:TYR:CB	2.47	0.44
6:B:1752:BOG:H5	6:B:1752:BOG:O2	2.18	0.44
1:A:229:ASP:HB3	1:B:139:TRP:CZ2	2.52	0.44
1:B:121[B]:SER:O	1:B:123[B]:LEU:O	2.36	0.44
1:B:413:MET:CE	4:B:1681:NAG:H61	2.48	0.44
1:A:281:PRO:HA	1:A:282:GLN:C	2.38	0.44
1:A:544:TYR:CE2	1:B:127[A]:PRO:HB2	2.53	0.44
1:A:235:GLY:HA3	1:A:236:ASP:HA	1.81	0.44
1:B:422:LEU:HA	1:B:422:LEU:HD12	1.84	0.44
1:B:422:LEU:O	1:B:426:PHE:CD2	2.71	0.44
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.99	0.44
1:B:206:THR:HA	1:B:209:PHE:CZ	2.53	0.44
1:A:290:GLU:C	1:A:291:VAL:CG2	2.87	0.44
1:A:330:GLN:HG2	1:B:138:SER:HB2	1.99	0.44
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.58	0.44
1:A:346:GLU:HG2	1:A:359:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:HA	1:B:220:PHE:O	2.18	0.43
1:B:381:PHE:O	1:B:385:TYR:HB2	2.18	0.43
1:A:422:LEU:O	1:A:426:PHE:CD2	2.72	0.43
3:A:674:BMA:C5	3:A:675:MAN:H2	2.46	0.43
1:A:129:THR:HG23	1:A:130:TYR:N	2.33	0.43
1:A:539:ILE:HA	1:A:544:TYR:CB	2.47	0.43
1:A:206:THR:HA	1:A:209:PHE:CZ	2.54	0.43
1:A:72:PRO:HB2	1:A:77:TRP:HB2	2.01	0.43
1:B:181:PHE:C	1:B:182:LEU:HD12	2.38	0.43
1:A:139:TRP:CZ2	1:B:229:ASP:HB3	2.53	0.43
1:A:183:LEU:O	1:A:438:ARG:HB2	2.19	0.43
1:A:58:ASP:OD2	1:B:546:LYS:HB3	2.18	0.43
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.48	0.43
1:B:38:TYR:CD1	4:B:1662:NDG:H8C2	2.53	0.43
1:A:181:PHE:C	1:A:182:LEU:HD12	2.38	0.43
1:A:461:GLN:HB3	1:A:462:PRO:HD2	2.01	0.43
1:A:272:LEU:C	1:A:272:LEU:HD23	2.38	0.43
1:B:107:PHE:HD1	1:B:108:ILE:N	2.17	0.43
3:A:673:MAN:HO6	3:A:674:BMA:HO2	1.65	0.43
1:B:391:MET:HA	1:B:392:PRO:HD3	1.84	0.43
1:B:458:LEU:HB2	1:B:460:LEU:CD1	2.49	0.43
1:A:381:PHE:O	1:A:385:TYR:HB2	2.18	0.43
1:B:461:GLN:HB3	1:B:462:PRO:HD2	2.01	0.43
1:B:127[B]:PRO:O	1:B:128[B]:PRO:C	2.57	0.43
1:A:502:GLU:HB2	1:A:505:PRO:HG2	2.00	0.43
1:B:302:ALA:HA	9:B:607:HOH:O	2.19	0.43
1:B:120[B]:ARG:HD3	6:B:1751:BOG:C6	2.46	0.42
1:B:272:LEU:HD23	1:B:272:LEU:C	2.39	0.42
1:A:458:LEU:HB2	1:A:460:LEU:CD1	2.49	0.42
1:A:289:GLN:HG3	1:A:292:PHE:CD1	2.54	0.42
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.00	0.42
1:A:107:PHE:HD1	1:A:108:ILE:N	2.16	0.42
1:B:152:LEU:HD12	1:B:466:TYR:CD1	2.55	0.42
1:B:125[B]:PRO:CB	1:B:372:GLN:H	2.32	0.42
1:A:161:THR:HG21	1:A:166:LYS:O	2.19	0.42
1:B:275:TYR:HB3	1:B:279:ILE:HD12	2.02	0.42
1:B:120[A]:ARG:NH1	1:B:524:GLU:OE2	2.50	0.42
1:B:161:THR:HG21	1:B:166:LYS:O	2.19	0.42
1:B:106:THR:HG22	1:B:107:PHE:H	1.84	0.42
4:A:681:NAG:O4	4:A:682:NDG:C7	2.67	0.42
2:A:601:HEM:CBD	2:A:601:HEM:HHA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLN:HG3	1:B:292:PHE:CD1	2.54	0.42
1:A:543[B]:GLU:CB	1:B:126[B]:SER:HB2	2.22	0.42
1:B:125[A]:PRO:HD3	1:B:151:ILE:CD1	2.49	0.42
1:B:129[A]:THR:CG2	1:B:130[A]:TYR:N	2.83	0.42
1:A:185:ARG:CZ	1:A:438:ARG:HH11	2.33	0.42
1:B:214:GLY:O	1:B:215:LYS:C	2.59	0.42
1:A:266:VAL:HG13	1:A:270:PRO:HA	2.01	0.42
1:B:481:LEU:O	1:B:511:LYS:HG3	2.20	0.41
3:A:673:MAN:O3	3:A:674:BMA:H61	2.20	0.41
1:B:391:MET:CE	2:B:601:HEM:HMC2	2.50	0.41
1:A:238:LEU:HD21	1:A:242:TYR:CZ	2.55	0.41
1:A:139:TRP:CZ2	1:B:229:ASP:CB	3.03	0.41
1:B:271:VAL:CG2	1:B:286:ALA:HB1	2.50	0.41
1:B:183:LEU:O	1:B:438:ARG:HB2	2.19	0.41
1:A:330:GLN:HG3	9:A:610:HOH:O	2.20	0.41
1:B:72:PRO:HB2	1:B:77:TRP:HB2	2.02	0.41
1:A:345:ILE:HD12	1:A:361:PHE:CD1	2.55	0.41
1:B:122[B]:ASN:C	1:B:123[B]:LEU:O	2.57	0.41
1:A:289:GLN:CG	1:A:292:PHE:CE1	3.03	0.41
1:B:205:PHE:O	1:B:205:PHE:CG	2.74	0.41
1:A:124:ILE:HD11	1:A:528:PRO:C	2.40	0.41
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.55	0.41
1:A:88:PHE:CE2	6:A:754:BOG:H7'1	2.56	0.41
1:B:124[A]:ILE:CG2	1:B:125[A]:PRO:CD	2.99	0.41
1:B:518:PHE:CG	1:B:522:MET:HG2	2.55	0.41
1:A:527:ALA:N	1:A:528:PRO:CD	2.84	0.41
1:A:387:TRP:CB	1:A:390:LEU:HD12	2.51	0.41
1:A:344:VAL:HG11	1:A:534:LEU:HD21	2.03	0.41
1:A:396:ARG:HG3	1:A:397:VAL:N	2.36	0.41
1:B:130[B]:TYR:HB2	1:B:150:ARG:HG2	2.02	0.41
1:B:410:ASN:ND2	4:B:1681:NAG:O5	2.48	0.40
1:A:192:GLN:HB3	1:A:192:GLN:HE21	1.61	0.40
1:B:464:ASN:HB3	1:B:474:PRO:HB3	2.03	0.40
1:B:344:VAL:HG11	1:B:534:LEU:HD21	2.03	0.40
1:A:280:PRO:C	1:A:281:PRO:O	2.53	0.40
1:B:289:GLN:CG	1:B:292:PHE:CE1	3.03	0.40
1:A:254:TYR:N	1:A:264:PRO:HG3	2.36	0.40
1:B:115:LEU:O	1:B:119:VAL:CB	2.66	0.40
1:B:523:ILE:HD11	5:B:1701:CEL:O2	2.21	0.40
1:B:527:ALA:N	1:B:528:PRO:CD	2.83	0.40
1:B:254:TYR:N	1:B:264:PRO:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:344:VAL:HG23	2.22	0.40
1:A:290:GLU:H	1:A:290:GLU:CD	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ILE:O	4:A:681:NAG:H83[4_565]	1.56	0.04

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	552/553 (100%)	508 (92%)	41 (7%)	3 (0%)	34	67
1	B	563/553 (102%)	507 (90%)	54 (10%)	2 (0%)	39	72
All	All	1115/1106 (101%)	1015 (91%)	95 (8%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	462	PRO
1	B	462	PRO
1	B	399	PRO
1	A	160	PRO

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	462/488 (95%)	451 (98%)	11 (2%)	57 86
1	B	472/488 (97%)	457 (97%)	15 (3%)	46 78
All	All	934/976 (96%)	908 (97%)	26 (3%)	51 82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	A	180	ARG
1	A	290	GLU
1	A	291	VAL
1	A	347	GLU
1	A	380	GLU
1	A	383	GLN
1	A	385	TYR
1	A	390	LEU
1	A	438	ARG
1	A	518	PHE
1	B	106	THR
1	B	107	PHE
1	B	144	ASN
1	B	158	ASP
1	B	213	SER
1	B	291	VAL
1	B	380	GLU
1	B	383	GLN
1	B	385	TYR
1	B	390	LEU
1	B	422	LEU
1	B	438	ARG
1	B	508	LEU
1	B	511	LYS
1	B	518	PHE

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	90	HIS

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	370	GLN
1	B	68	ASN
1	B	192	GLN
1	B	320	HIS
1	B	370	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

15 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	3	14,14,15	0.98	1 (7%)	15,19,21	1.74	4 (26%)
3	NAG	A	672	3	14,14,15	1.18	1 (7%)	15,19,21	2.35	5 (33%)
3	MAN	A	673	3	11,11,12	0.84	0	14,15,17	2.38	5 (35%)
3	BMA	A	674	3	11,11,12	0.85	0	14,15,17	2.13	6 (42%)
3	MAN	A	675	3	11,11,12	0.61	0	14,15,17	0.86	1 (7%)
4	NAG	A	681	4	14,14,15	1.10	1 (7%)	15,19,21	1.54	1 (6%)
4	NDG	A	682	4	14,14,15	1.70	4 (28%)	15,19,21	2.14	4 (26%)
4	NAG	B	1661	4	14,14,15	1.16	1 (7%)	15,19,21	2.26	3 (20%)
4	NDG	B	1662	4	14,14,15	0.85	0	15,19,21	2.24	7 (46%)
8	NAG	B	1671	8	14,14,15	1.22	1 (7%)	15,19,21	1.80	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	B	1672	8	14,14,15	0.81	1 (7%)	15,19,21	2.12	3 (20%)
8	MAN	B	1673	8	11,11,12	0.69	0	14,15,17	1.77	4 (28%)
8	BMA	B	1674	8	11,11,12	1.04	1 (9%)	14,15,17	1.80	4 (28%)
4	NAG	B	1681	4	14,14,15	0.84	0	15,19,21	1.77	4 (26%)
4	NDG	B	1682	4	14,14,15	1.49	2 (14%)	15,19,21	1.94	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
3	NAG	A	671	3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	MAN	A	673	3	-	0/2/19/22	1/1/1/1
3	BMA	A	674	3	-	0/2/19/22	1/1/1/1
3	MAN	A	675	3	-	0/2/19/22	1/1/1/1
4	NAG	A	681	4	-	0/6/23/26	0/1/1/1
4	NDG	A	682	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1661	4	-	0/6/23/26	0/1/1/1
4	NDG	B	1662	4	-	0/6/23/26	0/1/1/1
8	NAG	B	1671	8	-	0/6/23/26	0/1/1/1
8	NAG	B	1672	8	-	0/6/23/26	0/1/1/1
8	MAN	B	1673	8	-	0/2/19/22	1/1/1/1
8	BMA	B	1674	8	-	0/2/19/22	1/1/1/1
4	NAG	B	1681	4	-	0/6/23/26	0/1/1/1
4	NDG	B	1682	4	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	672	NAG	O5-C1	-3.03	1.38	1.43
4	A	682	NDG	O-C1	-2.85	1.39	1.43
4	A	682	NDG	C1-C2	-2.75	1.48	1.52
4	B	1682	NDG	O-C1	-2.61	1.39	1.43
8	B	1671	NAG	O5-C1	-2.58	1.39	1.43
8	B	1674	BMA	O5-C1	-2.46	1.39	1.43
4	A	681	NAG	O5-C1	-2.30	1.39	1.43
4	B	1661	NAG	C2-N2	-2.30	1.42	1.46
3	A	671	NAG	O5-C1	-2.26	1.39	1.43
4	B	1682	NDG	O-C5	-2.25	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	682	NDG	C4-C5	-2.11	1.48	1.53
4	A	682	NDG	C2-N2	-2.11	1.42	1.46
8	B	1672	NAG	O5-C1	-2.10	1.40	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1661	NAG	C4-C3-C2	-6.19	101.60	111.23
4	B	1682	NDG	C4-C3-C2	-5.86	102.12	111.23
8	B	1672	NAG	C4-C3-C2	-5.21	103.13	111.23
3	A	673	MAN	C3-C4-C5	-5.03	101.42	110.20
3	A	672	NAG	C2-N2-C7	-4.64	117.08	123.04
3	A	672	NAG	O4-C4-C3	-4.56	100.08	110.34
3	A	673	MAN	C2-C3-C4	-4.42	103.54	111.04
4	B	1662	NDG	C4-C3-C2	-4.21	104.69	111.23
4	B	1662	NDG	C3-C4-C5	-4.15	102.95	110.20
4	B	1681	NAG	C2-N2-C7	-4.06	117.82	123.04
4	A	682	NDG	C3-C4-C5	-3.83	103.52	110.20
4	A	681	NAG	C3-C4-C5	-3.77	103.62	110.20
4	B	1661	NAG	C3-C4-C5	-3.77	103.63	110.20
3	A	672	NAG	C6-C5-C4	-3.73	103.81	113.02
3	A	673	MAN	O5-C1-C2	-3.64	104.95	110.86
4	A	682	NDG	C2-N2-C7	-3.54	118.49	123.04
3	A	674	BMA	C3-C4-C5	-3.53	104.04	110.20
3	A	674	BMA	C2-C3-C4	-3.45	105.19	111.04
3	A	674	BMA	O6-C6-C5	-3.43	100.01	111.33
8	B	1671	NAG	O4-C4-C3	-3.29	102.92	110.34
3	A	671	NAG	C6-C5-C4	-3.22	105.07	113.02
3	A	672	NAG	O5-C5-C6	-3.21	100.41	107.35
8	B	1674	BMA	C6-C5-C4	-3.04	105.52	113.02
8	B	1673	MAN	C2-C3-C4	-3.03	105.89	111.04
4	B	1681	NAG	C4-C3-C2	-3.00	106.57	111.23
3	A	671	NAG	C4-C3-C2	-2.96	106.63	111.23
3	A	674	BMA	O5-C5-C6	-2.92	101.02	107.35
8	B	1671	NAG	O3-C3-C4	-2.90	103.81	110.34
8	B	1673	MAN	C3-C4-C5	-2.81	105.30	110.20
4	B	1662	NDG	C6-C5-C4	-2.81	106.09	113.02
4	B	1661	NAG	C6-C5-C4	-2.80	106.12	113.02
8	B	1674	BMA	O6-C6-C5	-2.75	102.25	111.33
8	B	1673	MAN	O2-C2-C3	-2.68	104.72	110.12
8	B	1674	BMA	C2-C3-C4	-2.67	106.50	111.04
3	A	673	MAN	C1-C2-C3	-2.67	106.39	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1671	NAG	C3-C4-C5	-2.66	105.56	110.20
4	B	1682	NDG	C2-N2-C7	-2.59	119.72	123.04
4	A	682	NDG	C4-C3-C2	-2.57	107.24	111.23
8	B	1671	NAG	C6-C5-C4	-2.56	106.70	113.02
4	B	1662	NDG	O7-C7-C8	-2.55	117.38	122.06
4	B	1662	NDG	O3-C3-C4	-2.53	104.65	110.34
3	A	674	BMA	O2-C2-C1	-2.43	104.33	109.21
8	B	1672	NAG	O5-C5-C6	-2.41	102.12	107.35
3	A	671	NAG	O4-C4-C3	-2.36	105.02	110.34
8	B	1674	BMA	O4-C4-C3	-2.35	105.06	110.34
3	A	671	NAG	O6-C6-C5	-2.34	103.60	111.33
3	A	674	BMA	C1-C2-C3	-2.23	106.91	109.54
4	B	1681	NAG	C6-C5-C4	-2.22	107.54	113.02
3	A	675	MAN	C2-C3-C4	-2.15	107.39	111.04
3	A	673	MAN	O2-C2-C3	-2.11	105.87	110.12
4	B	1662	NDG	O6-C6-C5	-2.08	104.45	111.33
3	A	672	NAG	C3-C4-C5	2.32	114.24	110.20
8	B	1672	NAG	C1-O5-C5	2.40	115.30	112.25
4	B	1662	NDG	C2-N2-C7	2.56	126.33	123.04
4	B	1681	NAG	C1-O5-C5	2.72	115.70	112.25
8	B	1673	MAN	C1-O5-C5	3.03	116.09	112.25
4	B	1682	NDG	C1-O-C5	3.19	116.30	112.25
4	A	682	NDG	C1-O-C5	4.42	117.86	112.25

There are no chirality outliers.

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	675	MAN	C1-C2-C3-C4-C5-O5
8	B	1673	MAN	C1-C2-C3-C4-C5-O5
8	B	1674	BMA	C1-C2-C3-C4-C5-O5
3	A	674	BMA	C1-C2-C3-C4-C5-O5
3	A	673	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	671	NAG	7	0
3	A	672	NAG	3	0
3	A	673	MAN	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	674	BMA	20	0
3	A	675	MAN	12	0
4	A	681	NAG	2	1
4	A	682	NDG	1	0
4	B	1661	NAG	5	0
4	B	1662	NDG	5	0
8	B	1671	NAG	5	0
8	B	1672	NAG	6	0
8	B	1673	MAN	2	0
8	B	1674	BMA	2	0
4	B	1681	NAG	9	0
4	B	1682	NDG	3	0

5.6 Ligand geometry (i)

9 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	-	30,50,50	2.21	8 (26%)	24,82,82	2.29	7 (29%)
5	CEL	A	701	-	27,28,28	3.58	10 (37%)	40,43,43	1.98	8 (20%)
6	BOG	A	751	-	20,20,20	0.87	1 (5%)	25,25,25	1.83	5 (20%)
6	BOG	A	754	-	20,20,20	0.91	1 (5%)	25,25,25	1.75	5 (20%)
7	FLC	A	900	-	3,12,12	2.85	2 (66%)	3,17,17	3.12	2 (66%)
5	CEL	B	1701	-	27,28,28	3.91	11 (40%)	40,43,43	2.22	12 (30%)
6	BOG	B	1751	-	20,20,20	1.32	4 (20%)	25,25,25	2.08	6 (24%)
6	BOG	B	1752	-	20,20,20	0.84	1 (5%)	25,25,25	2.76	5 (20%)
2	HEM	B	601	-	30,50,50	2.24	11 (36%)	24,82,82	2.23	6 (25%)

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	-	-	0/10/54/54	0/0/8/8
5	CEL	A	701	-	-	0/20/20/20	0/3/3/3
6	BOG	A	751	-	-	0/11/31/31	0/1/1/1
6	BOG	A	754	-	-	0/11/31/31	0/1/1/1
7	FLC	A	900	-	-	0/6/16/16	0/0/0/0
5	CEL	B	1701	-	-	0/20/20/20	0/3/3/3
6	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
6	BOG	B	1752	-	1/1/5/5	0/11/31/31	0/1/1/1
2	HEM	B	601	-	-	0/10/54/54	0/0/8/8

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	-7.30	1.45	1.51
2	B	601	HEM	C3B-C4B	-7.17	1.45	1.51
5	A	701	CEL	C2-C1	-6.41	1.31	1.39
5	B	1701	CEL	C2-C1	-6.40	1.31	1.39
2	B	601	HEM	C3D-C4D	-5.34	1.44	1.51
2	A	601	HEM	C3D-C4D	-5.19	1.44	1.51
7	A	900	FLC	OHB-CB	-3.90	1.36	1.43
2	B	601	HEM	C2C-C1C	-3.89	1.45	1.52
2	A	601	HEM	C2C-C1C	-3.79	1.45	1.52
6	B	1751	BOG	O5-C5	-3.63	1.35	1.44
7	A	900	FLC	CA-CB	-2.87	1.50	1.54
5	B	1701	CEL	C10-C5	-2.86	1.33	1.39
5	A	701	CEL	C10-C5	-2.86	1.33	1.39
6	B	1751	BOG	O5-C1	-2.66	1.35	1.41
5	B	1701	CEL	C14-C15	-2.56	1.34	1.38
5	A	701	CEL	C14-C15	-2.55	1.34	1.38
5	B	1701	CEL	C6-C7	-2.50	1.34	1.38
5	A	701	CEL	C6-C7	-2.46	1.34	1.38
6	A	754	BOG	O5-C5	-2.33	1.38	1.44
5	B	1701	CEL	C16-C17	-2.28	1.34	1.38
6	B	1751	BOG	C1-C2	-2.24	1.45	1.52
5	A	701	CEL	C16-C17	-2.24	1.34	1.38
6	A	751	BOG	O5-C5	-2.21	1.38	1.44
6	B	1751	BOG	O2-C2	-2.20	1.37	1.43
6	B	1752	BOG	O5-C5	-2.17	1.38	1.44
2	A	601	HEM	C2D-C1D	-2.08	1.45	1.51
2	B	601	HEM	C2D-C1D	-2.08	1.45	1.51
2	A	601	HEM	C2B-C1B	-2.05	1.45	1.51
2	B	601	HEM	C2B-C1B	-2.03	1.45	1.51
2	A	601	HEM	C3C-CAC	2.04	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-CAB	2.05	1.55	1.51
2	B	601	HEM	C3C-CAC	2.06	1.55	1.51
2	B	601	HEM	FE-ND	2.11	2.08	1.97
2	B	601	HEM	C3B-CAB	2.11	1.55	1.51
2	B	601	HEM	C1C-NC	2.17	1.38	1.36
2	B	601	HEM	C4C-NC	2.33	1.38	1.36
5	B	1701	CEL	C6-C5	2.69	1.45	1.39
5	A	701	CEL	C6-C5	2.69	1.45	1.39
2	A	601	HEM	FE-NC	2.75	2.06	1.95
2	B	601	HEM	FE-NC	2.76	2.06	1.95
5	B	1701	CEL	S1-N3	2.97	1.67	1.60
5	A	701	CEL	S1-N3	3.32	1.67	1.60
5	A	701	CEL	C16-C15	4.63	1.46	1.38
5	B	1701	CEL	C16-C15	4.65	1.46	1.38
5	B	1701	CEL	C15-S1	9.29	1.91	1.77
5	B	1701	CEL	O2-S1	9.75	1.60	1.43
5	A	701	CEL	O2-S1	10.42	1.61	1.43
5	B	1701	CEL	O1-S1	10.65	1.62	1.43
5	A	701	CEL	O1-S1	10.77	1.62	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	701	CEL	O1-S1-O2	-6.19	110.11	118.80
6	B	1751	BOG	O5-C1-C2	-5.75	98.47	110.28
6	A	754	BOG	O5-C1-C2	-4.96	100.09	110.28
6	B	1752	BOG	C1'-O1-C1	-4.96	105.27	113.94
7	A	900	FLC	CB-CA-CAC	-4.89	107.14	114.96
6	B	1751	BOG	O2-C2-C1	-4.63	99.87	110.02
6	A	751	BOG	O5-C1-C2	-4.53	100.98	110.28
5	B	1701	CEL	O1-S1-O2	-4.18	112.92	118.80
6	A	751	BOG	C4-C3-C2	-4.05	103.24	110.79
6	A	751	BOG	C1'-O1-C1	-4.00	106.96	113.94
5	B	1701	CEL	C15-S1-N3	-3.74	103.50	108.45
6	B	1751	BOG	O1-C1-C2	-3.44	103.69	108.04
6	B	1751	BOG	O5-C5-C6	-3.39	97.79	106.36
6	A	754	BOG	O5-C5-C4	-3.30	103.48	109.68
5	B	1701	CEL	C16-C15-S1	-3.25	114.45	119.74
6	A	754	BOG	C4-C3-C2	-3.24	104.74	110.79
6	A	751	BOG	O5-C5-C4	-3.19	103.70	109.68
6	B	1752	BOG	O5-C5-C4	-3.14	103.80	109.68
6	A	754	BOG	C1-C2-C3	-2.67	104.71	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1751	BOG	C1-O5-C5	-2.50	108.90	113.75
6	A	754	BOG	C3-C4-C5	-2.49	105.86	110.20
5	B	1701	CEL	C2-C3-C5	-2.42	124.10	128.12
5	A	701	CEL	C2-C3-C5	-2.39	124.15	128.12
6	A	751	BOG	C1-C2-C3	-2.36	105.33	109.97
5	B	1701	CEL	F2-C4-C1	-2.13	108.77	112.55
5	A	701	CEL	F2-C4-C1	-2.13	108.77	112.55
5	A	701	CEL	C2-C1-N1	-2.08	108.26	111.53
5	B	1701	CEL	C2-C1-N1	-2.08	108.27	111.53
2	A	601	HEM	C3B-C4B-CHC	2.04	126.04	123.16
6	B	1752	BOG	O5-C1-C2	2.05	114.48	110.28
5	B	1701	CEL	C3-C2-C1	2.13	107.58	104.81
5	A	701	CEL	C3-C2-C1	2.18	107.63	104.81
7	A	900	FLC	CG-CB-CA	2.19	115.05	109.81
5	B	1701	CEL	O1-S1-N3	2.42	110.42	107.28
2	B	601	HEM	C2D-C3D-C4D	2.49	105.71	101.50
2	A	601	HEM	C2D-C3D-C4D	2.50	105.73	101.50
2	A	601	HEM	CMD-C2D-C3D	2.84	126.91	114.35
5	A	701	CEL	C5-C3-N2	2.88	128.21	123.23
5	B	1701	CEL	C5-C3-N2	2.89	128.22	123.23
2	B	601	HEM	CMD-C2D-C3D	2.96	127.44	114.35
5	B	1701	CEL	C14-C15-S1	3.42	125.31	119.74
6	B	1751	BOG	C3-C4-C5	3.52	116.33	110.20
2	B	601	HEM	CMC-C2C-C3C	3.56	125.43	116.53
2	B	601	HEM	CAD-C3D-C4D	4.00	126.59	112.47
2	A	601	HEM	CAD-C3D-C4D	4.31	127.68	112.47
5	A	701	CEL	C4-C1-N1	4.55	125.38	119.65
5	B	1701	CEL	C4-C1-N1	4.58	125.41	119.65
2	A	601	HEM	CAD-C3D-C2D	4.65	126.59	113.22
2	A	601	HEM	CMC-C2C-C3C	4.74	128.36	116.53
2	B	601	HEM	CMB-C2B-C3B	4.84	128.60	116.53
2	A	601	HEM	CMB-C2B-C3B	4.89	128.73	116.53
2	B	601	HEM	CAD-C3D-C2D	5.03	127.68	113.22
6	B	1752	BOG	O5-C1-O1	6.13	124.82	110.05
5	A	701	CEL	O2-S1-N3	6.14	115.23	107.28
5	B	1701	CEL	O2-S1-C15	7.70	116.88	107.39
6	B	1752	BOG	O1-C1-C2	10.02	120.70	108.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1752	BOG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	7	0
5	A	701	CEL	9	0
6	A	751	BOG	1	0
6	A	754	BOG	3	0
5	B	1701	CEL	8	0
6	B	1751	BOG	12	0
6	B	1752	BOG	1	0
2	B	601	HEM	10	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	553/553 (100%)	0.34	14 (2%)	61	54	52, 87, 130, 213	0
1	B	553/553 (100%)	0.35	20 (3%)	46	40	54, 86, 129, 195	3 (0%)
All	All	1106/1106 (100%)	0.35	34 (3%)	52	46	52, 86, 130, 213	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	3.7
1	B	69	CYS	3.2
1	B	277	ARG	3.1
1	B	291	VAL	3.1
1	A	409	PHE	3.0
1	A	370	GLN	3.0
1	A	276	PRO	3.0
1	B	35	PRO	2.9
1	B	496	GLY	2.9
1	A	291	VAL	2.8
1	A	281	PRO	2.8
1	B	484	GLU	2.7
1	A	74	ILE	2.7
1	A	404	TYR	2.7
1	B	72	PRO	2.6
1	B	151	ILE	2.6
1	B	145	VAL	2.5
1	B	482	THR	2.5
1	A	151	ILE	2.5
1	A	200	PHE	2.4
1	B	107	PHE	2.4
1	B	489	ALA	2.4
1	B	488	ALA	2.3
1	A	482	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	123[A]	LEU	2.3
1	B	580	PHE	2.3
1	B	105	ALA	2.2
1	B	319	GLU	2.2
1	B	279	ILE	2.2
1	B	70	THR	2.2
1	A	258	ASN	2.1
1	B	106	THR	2.1
1	A	235	GLY	2.1
1	A	102	PHE	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	B	1661	14/15	0.96	0.18	-0.66	75,78,108,120	12
4	NAG	B	1681	14/15	0.93	0.16	-0.74	57,106,129,135	12
4	NDG	A	682	14/15	0.95	0.15	-0.90	79,79,140,146	13
4	NAG	A	681	14/15	0.92	0.15	-1.17	74,77,135,153	12
8	NAG	B	1672	14/15	0.93	0.14	-1.22	75,101,137,158	12
3	NAG	A	671	14/15	0.97	0.15	-1.28	34,53,80,93	12
8	NAG	B	1671	14/15	0.97	0.15	-1.37	46,77,96,110	12
3	NAG	A	672	14/15	0.94	0.15	-1.57	59,83,131,146	12
8	MAN	B	1673	11/12	0.88	0.10	-	78,164,171,176	6
3	MAN	A	675	11/12	0.91	0.13	-	100,141,159,165	0
3	BMA	A	674	11/12	0.83	0.12	-	74,88,182,186	9
8	BMA	B	1674	11/12	0.92	0.15	-	72,72,163,167	10
4	NDG	B	1682	14/15	0.89	0.24	-	70,70,181,190	13
4	NDG	B	1662	14/15	0.92	0.17	-	97,97,134,141	13
3	MAN	A	673	11/12	0.90	0.14	-	168,175,190,195	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^{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
5	CEL	B	1701	26/26	0.95	0.36	4.95	22,52,65,66	40
6	BOG	B	1751	20/20	0.96	0.21	0.62	37,68,111,134	28
6	BOG	A	751	20/20	0.92	0.20	0.44	67,78,129,150	30
7	FLC	A	900	13/13	0.87	0.18	-0.15	61,143,174,180	6
2	HEM	B	601	43/43	0.96	0.19	-0.26	45,78,116,157	30
2	HEM	A	601	43/43	0.96	0.18	-0.71	28,51,126,149	32
5	CEL	A	701	26/26	0.97	0.16	-0.75	49,77,95,121	14
6	BOG	B	1752	20/20	0.90	0.17	-1.40	70,70,156,159	28
6	BOG	A	754	20/20	0.90	0.15	-1.58	68,80,130,136	28

6.5 Other polymers

There are no such residues in this entry.