



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:18 AM GMT

PDB ID : 1CVU  
Title : CRYSTAL STRUCTURE OF ARACHIDONIC ACID BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2  
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.  
Deposited on : 1999-08-24  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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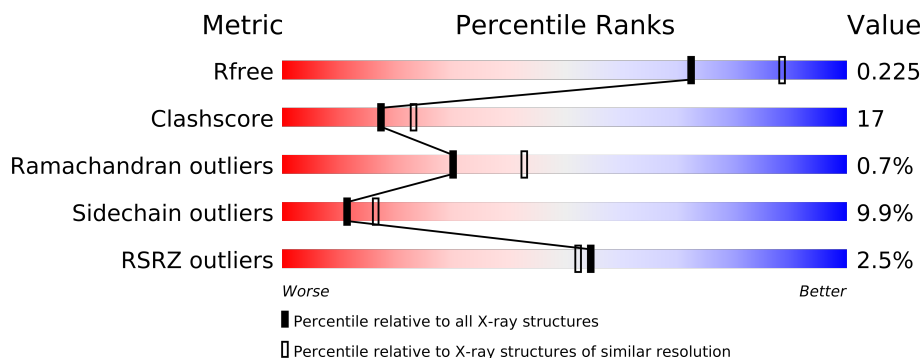
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	
2	F	9	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H2 SYNTHASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	ENGINEERED	UNP Q05769
A	333	LYS	ARG	ENGINEERED	UNP Q05769
B	2310	GLN	ASN	ENGINEERED	UNP Q05769
B	2333	LYS	ARG	ENGINEERED	UNP Q05769

- Molecule 2 is a protein called PROTEIN (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	9	Total	C	N	O	0	0	0
			63	37	11	15			

- 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		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	ENGINEERED	UNP Q05769
A	333	LYS	ARG	ENGINEERED	UNP Q05769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2310	GLN	ASN	ENGINEERED	UNP Q05769
B	2333	LYS	ARG	ENGINEERED	UNP Q05769

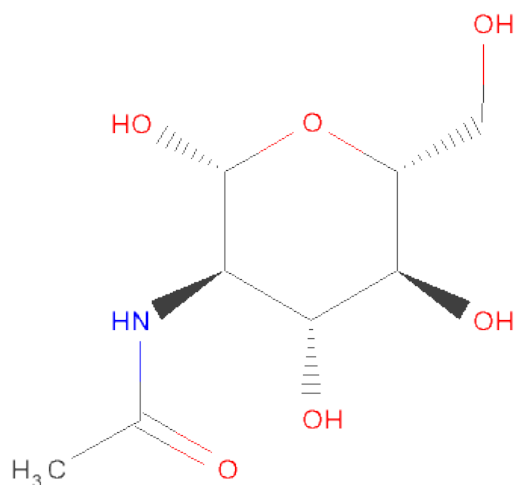
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		
4	B	4	Total	C	N	O	0	0
			50	28	2	20		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	ENGINEERED	UNP Q05769
A	333	LYS	ARG	ENGINEERED	UNP Q05769
B	2310	GLN	ASN	ENGINEERED	UNP Q05769
B	2333	LYS	ARG	ENGINEERED	UNP Q05769

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



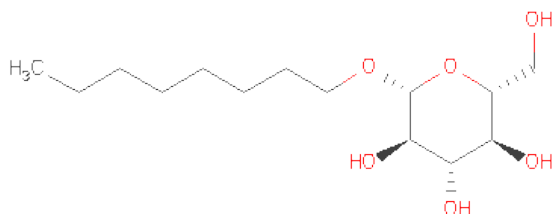
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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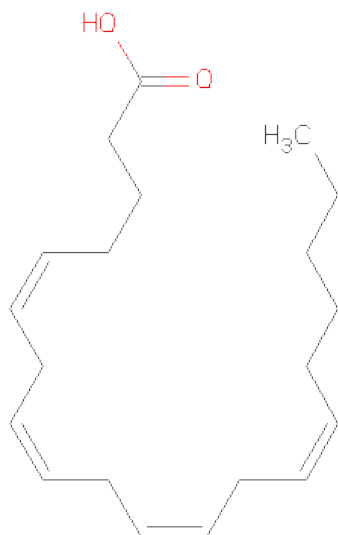
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 7 is ARACHIDONIC ACID (three-letter code: ACD) (formula:  $C_{20}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			22	20	2		
7	B	1	Total	C	O	0	0
			22	20	2		

- Molecule 8 is water.

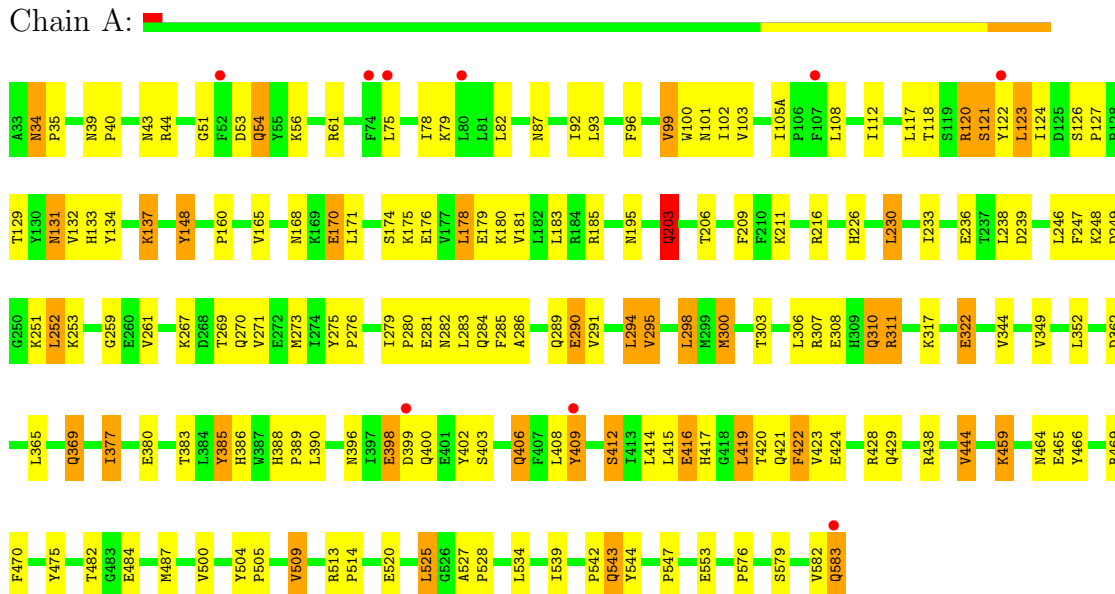
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	410	Total	O	0	0
			410	410		
8	B	361	Total	O	0	0
			361	361		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

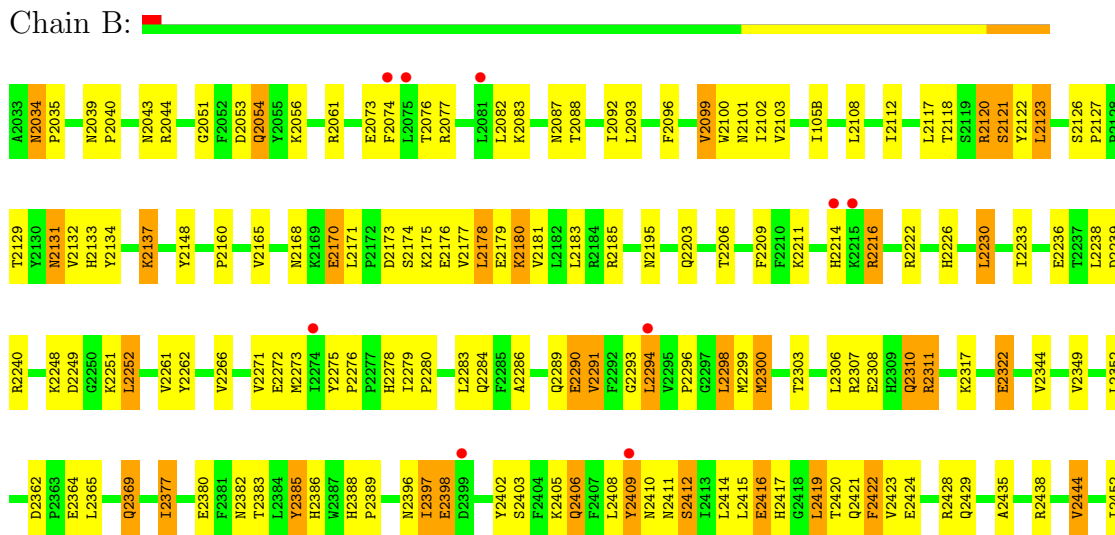
#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-2

Chain A:



#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-2

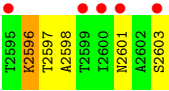
Chain B:





● Molecule 2: PROTEIN (9-MER)

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.04Å 133.96Å 124.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 34.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (35.00-2.40) 96.2 (34.95-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.235 0.198 , 0.225	Depositor DCC
$R_{free}$ test set	3887 reflections (7.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57179 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACD, BOG, NAG, 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	0.49	3/4595 (0.1%)	0.65	1/6229 (0.0%)
1	B	0.49	2/4595 (0.0%)	0.68	2/6229 (0.0%)
2	F	1.87	2/62 (3.2%)	1.70	2/82 (2.4%)
All	All	0.51	7/9252 (0.1%)	0.68	5/12540 (0.0%)

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	A	0	1
4	A	1	0
4	B	1	0
All	All	2	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2603	SER	C-O	9.63	1.41	1.23
2	F	2603	SER	C-OXT	-7.12	1.09	1.23
1	A	203	GLN	CD-OE1	5.84	1.36	1.24
1	B	2170	GLU	CD-OE2	5.66	1.31	1.25
1	B	2170	GLU	CD-OE1	5.66	1.31	1.25
1	A	170	GLU	CD-OE1	5.62	1.31	1.25
1	A	170	GLU	CD-OE2	5.38	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2603	SER	CA-C-O	11.83	144.95	120.10
1	B	2216	ARG	NE-CZ-NH1	-9.59	115.50	120.30
2	F	2603	SER	N-CA-C	6.91	129.66	111.00
1	B	2216	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	148	TYR	N-CA-C	-5.18	97.01	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	674	MAN	C1
4	B	2674	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4469	0	4373	154	0
1	B	4469	0	4373	163	0
2	F	63	0	65	8	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	50	0	42	3	0
4	B	50	0	42	5	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	60	0	84	6	0
6	B	40	0	56	6	0
7	A	22	0	31	0	0
7	B	22	0	31	0	0
8	A	410	0	0	8	0
8	B	361	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10100	0	9173	321	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (321) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2251:LYS:HD3	1:B:2310:GLN:HG3	1.49	0.92
1:A:251:LYS:HD3	1:A:310:GLN:HG3	1.51	0.89
1:B:2408:LEU:O	1:B:2409:TYR:HB2	1.74	0.87
1:B:2283:LEU:HD21	1:B:2415:LEU:HD12	1.55	0.85
1:A:543:GLN:HA	1:A:543:GLN:OE1	1.77	0.85
1:B:2209:PHE:HB2	1:B:2377:ILE:HD13	1.59	0.83
1:B:2543:GLN:OE1	1:B:2543:GLN:HA	1.77	0.83
1:A:209:PHE:HB2	1:A:377:ILE:HD13	1.60	0.81
1:A:246:LEU:HG	1:A:248:LYS:HG3	1.64	0.79
1:B:2216:ARG:NH1	4:B:2672:NAG:C7	2.47	0.78
1:A:300:MET:HE3	1:A:422:PHE:HB3	1.66	0.76
1:A:75:LEU:HD11	1:A:79:LYS:HE3	1.68	0.76
1:B:2275:TYR:HB3	1:B:2279:ILE:HD13	1.68	0.76
1:B:2300:MET:HE3	1:B:2422:PHE:HB3	1.66	0.76
2:F:2597:THR:HG22	2:F:2601:ASN:HD22	1.52	0.75
1:B:2464:ASN:HD21	1:B:2475:TYR:H	1.36	0.74
2:F:2597:THR:CG2	2:F:2601:ASN:ND2	2.51	0.73
1:A:51:GLY:C	1:B:2322:GLU:HG2	2.10	0.72
1:B:2209:PHE:HB2	1:B:2377:ILE:CD1	2.19	0.71
1:A:464:ASN:HD21	1:A:475:TYR:H	1.37	0.71
2:F:2597:THR:HG23	2:F:2601:ASN:HD21	1.54	0.70
1:A:322:GLU:HG2	1:B:2051:GLY:C	2.11	0.70
1:A:129:THR:HG22	1:A:137:LYS:HD3	1.72	0.70
1:B:2582:VAL:HG13	1:B:2583:GLN:OE1	1.91	0.70
2:F:2597:THR:HG23	2:F:2601:ASN:ND2	2.07	0.69
1:A:209:PHE:HB2	1:A:377:ILE:CD1	2.22	0.69
1:B:2129:THR:HG22	1:B:2137:LYS:HD3	1.76	0.68
1:A:582:VAL:HG13	1:A:583:GLN:OE1	1.92	0.68
1:A:412:SER:O	1:A:416:GLU:HB2	1.94	0.67
1:A:396:ASN:H	1:A:429:GLN:HE22	1.44	0.66
1:A:424:GLU:O	1:A:428:ARG:HG3	1.96	0.66
1:B:2276:PRO:O	1:B:2279:ILE:HD12	1.95	0.65
1:A:300:MET:CE	1:A:422:PHE:HB3	2.26	0.65
1:B:2061:ARG:HD2	8:B:3380:HOH:O	1.96	0.65
1:B:2131:ASN:C	1:B:2131:ASN:HD22	2.00	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2300:MET:CE	1:B:2422:PHE:HB3	2.26	0.65
1:B:2271:VAL:HG21	1:B:2286:ALA:HB1	1.77	0.64
1:A:185:ARG:HH11	6:A:703:BOG:H4'1	1.61	0.64
1:A:469:ARG:O	1:A:469:ARG:HD2	1.98	0.64
1:A:131:ASN:C	1:A:131:ASN:HD22	2.00	0.63
1:B:2414:LEU:HD11	1:B:2419:LEU:HD22	1.81	0.63
1:A:398:GLU:OE1	1:A:417:HIS:HD2	1.81	0.63
1:A:75:LEU:HD12	1:A:75:LEU:O	1.99	0.63
1:B:2293:GLY:HA2	1:B:2299:MET:CE	2.29	0.63
1:B:2283:LEU:HD21	1:B:2415:LEU:CD1	2.26	0.62
1:B:2527:ALA:HB3	1:B:2528:PRO:HD3	1.82	0.62
1:B:2424:GLU:O	1:B:2428:ARG:HG3	1.99	0.62
1:B:2216:ARG:HG2	4:B:2672:NAG:O7	1.98	0.62
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.82	0.62
1:A:543:GLN:HB2	8:A:3119:HOH:O	1.99	0.62
2:F:2597:THR:HG22	2:F:2601:ASN:ND2	2.14	0.61
1:B:2211:LYS:NZ	1:B:2236:GLU:HG2	2.15	0.61
1:A:251:LYS:CD	1:A:310:GLN:HG3	2.30	0.61
1:A:185:ARG:NH1	6:A:703:BOG:H4'1	2.16	0.61
1:A:444:VAL:HG13	1:A:444:VAL:O	1.99	0.61
1:A:273:MET:SD	1:A:290:GLU:HA	2.40	0.60
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.81	0.60
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.84	0.60
1:A:211:LYS:NZ	1:A:236:GLU:HG2	2.17	0.59
1:B:2203:GLN:HG2	1:B:2298:LEU:HD11	1.83	0.59
1:A:420:THR:HG23	1:A:576:PRO:HG3	1.84	0.59
1:B:2398:GLU:OE2	1:B:2421:GLN:HG2	2.02	0.59
1:B:2293:GLY:HA2	1:B:2299:MET:HE3	1.83	0.59
1:B:2251:LYS:CD	1:B:2310:GLN:HG3	2.29	0.59
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.85	0.59
1:B:2293:GLY:O	1:B:2411:ASN:ND2	2.30	0.58
1:B:2230:LEU:HD13	1:B:2233:ILE:HD12	1.84	0.58
1:B:2402:TYR:OH	1:B:2417:HIS:HE1	1.86	0.58
1:B:2053:ASP:C	1:B:2054:GLN:HG3	2.23	0.58
1:B:2280:PRO:HG2	1:B:2283:LEU:HD12	1.85	0.58
1:B:2482:THR:HG22	1:B:2509:VAL:HG13	1.86	0.58
1:A:203:GLN:OE1	6:A:704:BOG:H5'1	2.04	0.58
1:A:294:LEU:HA	1:A:409:TYR:CE2	2.37	0.58
1:B:2469:ARG:HD2	1:B:2469:ARG:O	2.03	0.58
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.69	0.58
1:B:2181:VAL:HG12	1:B:2487:MET:HG2	1.87	0.57
1:A:53:ASP:C	1:A:54:GLN:HG3	2.25	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2108:LEU:O	1:B:2112:ILE:HG12	2.04	0.57
1:B:105(B):ILE:HG22	1:B:2108:LEU:H	1.68	0.57
4:A:672:NAG:H61	4:A:673:MAN:C1	2.35	0.57
1:B:2310:GLN:HG2	8:B:3241:HOH:O	2.04	0.56
1:B:2148:TYR:HD1	1:B:2377:ILE:HG22	1.70	0.56
1:B:2364:GLU:HG3	8:B:3734:HOH:O	2.05	0.56
1:B:2383:THR:HA	1:B:2386:HIS:CD2	2.41	0.56
1:A:280:PRO:O	1:A:284:GLN:HG3	2.04	0.56
1:A:543:GLN:O	1:B:2137:LYS:HE2	2.07	0.55
1:A:108:LEU:O	1:A:112:ILE:HG12	2.06	0.55
1:B:2444:VAL:O	1:B:2444:VAL:HG13	2.06	0.55
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.41	0.55
1:A:137:LYS:HE2	1:B:2543:GLN:O	2.06	0.55
1:B:2211:LYS:NZ	1:B:2236:GLU:CG	2.69	0.55
1:A:195:ASN:HB3	1:A:582:VAL:HG23	1.89	0.55
1:B:2120:ARG:HG2	1:B:2120:ARG:HH11	1.71	0.55
4:B:2672:NAG:H61	4:B:2673:MAN:C1	2.37	0.55
1:B:2500:VAL:HG12	1:B:2500:VAL:O	2.07	0.55
1:B:2396:ASN:H	1:B:2429:GLN:HE22	1.55	0.54
1:B:2470:PHE:CG	1:B:2525:LEU:HD22	2.42	0.54
1:B:2420:THR:HG23	1:B:2576:PRO:HG3	1.89	0.54
1:B:2412:SER:O	1:B:2416:GLU:HB2	2.06	0.54
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.71	0.54
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.43	0.53
2:F:2596:LYS:HD2	2:F:2597:THR:H	1.73	0.53
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.70	0.53
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.39	0.53
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.91	0.53
1:B:2575:CYS:SG	2:F:2598:ALA:HA	2.49	0.53
1:B:2148:TYR:CD1	1:B:2377:ILE:HG22	2.43	0.53
1:B:2203:GLN:OE1	6:B:2704:BOG:H5'1	2.09	0.53
1:B:2403:SER:OG	1:B:2406:GLN:HG3	2.09	0.53
1:A:226:HIS:C	1:A:377:ILE:HD12	2.30	0.52
1:B:2195:ASN:HB3	1:B:2582:VAL:HG23	1.90	0.52
1:B:2271:VAL:O	1:B:2271:VAL:HG23	2.08	0.52
1:B:2226:HIS:C	1:B:2377:ILE:HD12	2.30	0.52
1:B:2175:LYS:O	1:B:2179:GLU:HG3	2.10	0.52
1:A:75:LEU:CD1	1:A:79:LYS:HG3	2.40	0.51
1:B:2276:PRO:HD2	1:B:2279:ILE:CD1	2.39	0.51
1:B:2582:VAL:O	1:B:2582:VAL:HG12	2.11	0.51
1:A:175:LYS:O	1:A:179:GLU:HG3	2.11	0.51
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:THR:O	1:A:270:GLN:HB2	2.10	0.51
1:B:2296:PRO:HG3	1:B:2410:ASN:O	2.10	0.51
1:B:2083:LYS:HE2	8:B:3296:HOH:O	2.10	0.51
1:A:465:GLU:HA	1:A:465:GLU:OE1	2.10	0.51
1:B:2504:TYR:HB3	1:B:2505:PRO:HD3	1.92	0.51
1:B:2276:PRO:HB2	1:B:2278:HIS:CE1	2.46	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.94	0.50
1:B:2240:ARG:NH2	1:B:2273:MET:CE	2.74	0.50
1:B:2102:ILE:HG13	1:B:2103:VAL:N	2.27	0.50
1:A:261:VAL:O	1:A:307:ARG:NH1	2.44	0.50
1:A:513:ARG:NH2	1:A:520:GLU:HG3	2.27	0.50
1:A:383:THR:HA	1:A:386:HIS:CD2	2.47	0.50
1:A:280:PRO:HB2	1:A:282:ASN:OD1	2.11	0.50
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.95	0.50
1:B:2039:ASN:N	1:B:2040:PRO:CD	2.75	0.49
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.93	0.49
1:A:267:LYS:HD3	1:A:281:GLU:OE1	2.11	0.49
1:A:582:VAL:O	1:A:582:VAL:HG12	2.12	0.49
1:B:2034:ASN:C	1:B:2034:ASN:HD22	2.16	0.49
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.48	0.49
1:B:2291:VAL:O	1:B:2294:LEU:HG	2.13	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.93	0.49
1:B:2131:ASN:HD21	1:B:2134:TYR:HD1	1.61	0.49
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.48	0.49
1:A:179:GLU:OE2	6:A:703:BOG:H1	2.13	0.48
1:A:403:SER:OG	1:A:406:GLN:HG2	2.13	0.48
1:B:2121:SER:O	1:B:2123:LEU:N	2.46	0.48
1:A:121:SER:O	1:A:123:LEU:N	2.46	0.48
1:B:2294:LEU:N	1:B:2294:LEU:HD23	2.27	0.48
1:A:131:ASN:HD21	1:A:134:TYR:HD1	1.60	0.48
1:A:500:VAL:HG12	1:A:500:VAL:O	2.14	0.48
1:A:132:VAL:HG13	1:A:133:HIS:CD2	2.49	0.48
1:A:39:ASN:N	1:A:40:PRO:CD	2.77	0.48
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.13	0.48
1:A:102:ILE:HG13	1:A:103:VAL:N	2.26	0.48
1:B:2414:LEU:HA	1:B:2422:PHE:CE1	2.49	0.48
1:B:2174:SER:O	1:B:2178:LEU:HB2	2.13	0.48
1:B:2099:VAL:O	1:B:2102:ILE:HG12	2.14	0.47
1:A:421:GLN:HG2	8:A:3103:HOH:O	2.15	0.47
1:A:131:ASN:ND2	1:A:134:TYR:H	2.12	0.47
1:B:2102:ILE:CG1	1:B:2103:VAL:N	2.77	0.47
1:B:2275:TYR:O	1:B:2276:PRO:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:VAL:O	1:A:102:ILE:HG12	2.14	0.47
1:B:2126:SER:HA	1:B:2127:PRO:C	2.34	0.47
1:B:2465:GLU:HA	1:B:2465:GLU:OE1	2.14	0.47
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.48	0.47
1:A:174:SER:O	1:A:178:LEU:HB2	2.14	0.47
1:A:273:MET:HG3	1:A:285:PHE:O	2.14	0.47
1:A:294:LEU:HD23	1:A:295:VAL:HG23	1.97	0.47
1:A:295:VAL:CG2	1:A:298:LEU:HD22	2.44	0.47
1:A:34:ASN:C	1:A:34:ASN:HD22	2.17	0.47
1:A:43:ASN:O	1:A:44:ARG:HB2	2.15	0.47
1:A:547:PRO:HB3	1:A:553:GLU:OE1	2.14	0.47
1:B:2513:ARG:NH2	1:B:2520:GLU:HG3	2.30	0.47
1:B:2176:GLU:O	1:B:2180:LYS:HG3	2.15	0.46
1:B:2249:ASP:OD2	1:B:2317:LYS:HE2	2.15	0.46
1:B:2569:CYS:SG	2:F:2597:THR:HG22	2.55	0.46
1:A:303:THR:O	1:A:307:ARG:HD3	2.16	0.46
1:A:102:ILE:CG1	1:A:103:VAL:N	2.78	0.46
1:B:2262:TYR:CZ	1:B:2415:LEU:HD23	2.50	0.46
1:B:2386:HIS:CE1	6:B:2704:BOG:H1'2	2.51	0.46
1:A:126:SER:HA	1:A:127:PRO:C	2.36	0.46
1:A:176:GLU:O	1:A:180:LYS:HG3	2.16	0.46
1:B:2380:GLU:HG2	1:B:2466:TYR:CE1	2.51	0.46
1:B:2132:VAL:HG13	1:B:2133:HIS:CD2	2.51	0.46
1:B:2397:ILE:HD12	1:B:2422:PHE:CZ	2.51	0.46
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.29	0.46
1:A:226:HIS:HA	1:A:377:ILE:HD12	1.98	0.46
1:B:2419:LEU:O	1:B:2423:VAL:HG23	2.15	0.45
1:B:2290:GLU:H	1:B:2290:GLU:HG3	1.39	0.45
1:A:252:LEU:O	1:A:310:GLN:NE2	2.49	0.45
1:B:105(B):ILE:CG2	1:B:2108:LEU:HB2	2.46	0.45
1:B:2388:HIS:N	1:B:2389:PRO:CD	2.79	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.79	0.45
1:B:2547:PRO:HB3	1:B:2553:GLU:OE1	2.16	0.45
1:B:2464:ASN:HA	1:B:2464:ASN:HD22	1.61	0.45
1:B:2383:THR:HA	1:B:2386:HIS:HD2	1.80	0.45
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.99	0.45
1:B:2088:THR:HA	6:B:2702:BOG:H1'2	1.98	0.45
1:B:2131:ASN:ND2	1:B:2134:TYR:H	2.15	0.45
1:B:2397:ILE:HD12	1:B:2422:PHE:CE1	2.52	0.45
1:A:61:ARG:NH1	1:B:2542:PRO:O	2.50	0.45
1:B:2362:ASP:HB3	1:B:2365:LEU:HG	1.99	0.45
1:B:2226:HIS:HA	1:B:2377:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:459:LYS:HB3	1:A:459:LYS:HE2	1.63	0.45
1:B:2073:GLU:O	1:B:2076:THR:HB	2.16	0.45
1:B:2120:ARG:HD2	1:B:2120:ARG:HA	1.81	0.45
1:A:276:PRO:HG2	1:A:279:ILE:HD11	1.98	0.45
1:B:2298:LEU:HA	1:B:2298:LEU:HD12	1.86	0.45
1:B:2252:LEU:O	1:B:2310:GLN:NE2	2.49	0.44
1:B:2294:LEU:HB3	1:B:2409:TYR:CD2	2.51	0.44
1:A:419:LEU:O	1:A:423:VAL:HG23	2.16	0.44
1:A:306:LEU:HD23	1:A:306:LEU:C	2.37	0.44
1:B:2226:HIS:CA	1:B:2377:ILE:HD12	2.47	0.44
1:B:2240:ARG:NH2	1:B:2273:MET:HE1	2.32	0.44
1:A:61:ARG:NH2	8:A:3003:HOH:O	2.49	0.44
1:A:78:ILE:O	1:A:82:LEU:HD13	2.17	0.44
1:B:2276:PRO:HD2	1:B:2279:ILE:HD13	1.98	0.44
1:B:2293:GLY:HA2	1:B:2299:MET:HE1	1.97	0.44
4:A:672:NAG:C6	4:A:673:MAN:C1	2.96	0.44
4:B:2672:NAG:C6	4:B:2673:MAN:C1	2.95	0.44
1:B:2178:LEU:HD22	1:B:2183:LEU:HG	1.99	0.44
1:A:249:ASP:OD2	1:A:317:LYS:HE2	2.18	0.44
1:B:2308:GLU:OE1	1:B:2311:ARG:NH1	2.51	0.44
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.99	0.44
1:B:2180:LYS:HD3	1:B:2490:GLU:OE2	2.17	0.44
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.48	0.44
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.53	0.44
1:B:2459:LYS:HB3	1:B:2459:LYS:HE2	1.63	0.44
1:B:2216:ARG:HH11	4:B:2672:NAG:C7	2.27	0.43
1:B:2203:GLN:CG	1:B:2298:LEU:HD11	2.48	0.43
1:A:294:LEU:HD23	1:A:295:VAL:CG2	2.48	0.43
1:A:105(A):ILE:O	1:A:108:LEU:N	2.51	0.43
1:B:2405:LYS:HD2	8:B:3692:HOH:O	2.17	0.43
1:B:2088:THR:HG23	6:B:2702:BOG:H3'2	1.99	0.43
1:B:2266:VAL:HG23	1:B:2284:GLN:O	2.17	0.43
1:A:362:ASP:HB3	1:A:365:LEU:HG	2.00	0.43
1:B:2043:ASN:O	1:B:2044:ARG:HB2	2.18	0.43
1:B:2303:THR:O	1:B:2307:ARG:HD3	2.19	0.43
1:A:124:ILE:HB	8:A:3495:HOH:O	2.18	0.43
1:A:542:PRO:O	1:B:2061:ARG:NH1	2.51	0.43
1:B:2034:ASN:HD22	1:B:2035:PRO:N	2.16	0.43
1:A:34:ASN:HD22	1:A:35:PRO:N	2.16	0.43
1:B:2073:GLU:O	1:B:2074:PHE:C	2.56	0.43
1:B:2214:HIS:HD2	8:B:3233:HOH:O	2.02	0.43
1:B:2100:TRP:HA	1:B:2100:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:3106:HOH:O	1:B:2543:GLN:HB2	2.17	0.43
1:A:226:HIS:CA	1:A:377:ILE:HD12	2.48	0.43
1:A:247:PHE:C	1:A:248:LYS:HG2	2.39	0.43
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.19	0.43
1:B:2344:VAL:O	1:B:2349:VAL:HG23	2.19	0.43
1:A:553:GLU:HA	1:A:553:GLU:OE1	2.19	0.43
1:A:118:THR:HG22	1:A:369:GLN:HG2	2.00	0.43
1:B:2538:PRO:HD3	8:B:3638:HOH:O	2.17	0.43
1:B:2271:VAL:CG2	1:B:2273:MET:HE3	2.50	0.42
1:A:179:GLU:O	1:A:185:ARG:NH2	2.51	0.42
1:B:2087:ASN:HB3	6:B:2702:BOG:H3	2.01	0.42
1:B:2222:ARG:HD3	8:B:3289:HOH:O	2.19	0.42
1:A:276:PRO:HG2	1:A:279:ILE:HG13	2.01	0.42
1:B:2306:LEU:C	1:B:2306:LEU:HD23	2.38	0.42
1:B:105(B):ILE:O	1:B:2108:LEU:N	2.52	0.42
1:B:105(B):ILE:CD1	1:B:2108:LEU:HD12	2.48	0.42
1:B:2083:LYS:HE3	8:B:3661:HOH:O	2.18	0.42
1:A:131:ASN:HD22	1:A:134:TYR:H	1.67	0.42
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.49	0.42
1:B:2118:THR:HG22	1:B:2369:GLN:HG2	2.01	0.42
1:B:2160:PRO:HG2	1:B:2165:VAL:HA	2.01	0.42
1:A:396:ASN:H	1:A:429:GLN:NE2	2.15	0.42
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.82	0.42
1:A:183:LEU:O	1:A:438:ARG:HB3	2.20	0.42
1:A:400:GLN:HB2	1:A:402:TYR:CE2	2.55	0.42
1:A:283:LEU:HD21	1:A:415:LEU:HD12	2.02	0.42
1:A:275:TYR:HD2	1:A:279:ILE:HD12	1.84	0.42
1:A:464:ASN:ND2	1:A:475:TYR:H	2.11	0.42
1:A:294:LEU:HA	1:A:409:TYR:CD2	2.55	0.42
1:B:2470:PHE:CD2	1:B:2525:LEU:HD22	2.53	0.42
1:A:216:ARG:HH12	4:A:671:NAG:H3	1.84	0.42
1:A:398:GLU:HB3	1:A:399:ASP:H	1.68	0.42
1:A:280:PRO:HG2	1:A:283:LEU:HB2	2.02	0.42
1:B:2513:ARG:HD2	8:B:3249:HOH:O	2.19	0.42
1:B:2553:GLU:HA	1:B:2553:GLU:OE1	2.18	0.42
1:A:402:TYR:HA	1:A:406:GLN:OE1	2.20	0.42
1:A:259:GLY:N	8:A:3216:HOH:O	2.53	0.42
1:A:539:ILE:HA	1:A:544:TYR:HB3	2.02	0.42
1:B:2096:PHE:HB3	1:B:2099:VAL:HG13	2.01	0.41
1:B:2261:VAL:O	1:B:2307:ARG:NH1	2.50	0.41
1:A:276:PRO:HD2	1:A:279:ILE:HD12	2.02	0.41
1:B:2308:GLU:CD	1:B:2311:ARG:HH11	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2464:ASN:ND2	1:B:2475:TYR:H	2.10	0.41
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.84	0.41
1:B:2382:ASN:HD21	6:B:2704:BOG:H61	1.84	0.41
1:B:2082:LEU:N	1:B:2082:LEU:HD12	2.36	0.41
1:A:175:LYS:HG3	8:A:3497:HOH:O	2.20	0.41
1:B:2074:PHE:O	1:B:2077:ARG:HB2	2.20	0.41
1:B:2500:VAL:CG1	1:B:2500:VAL:O	2.68	0.41
1:A:96:PHE:HB3	1:A:99:VAL:HG13	2.01	0.41
1:A:253:LYS:HD3	8:A:3621:HOH:O	2.21	0.41
1:B:2554:VAL:HB	8:B:3346:HOH:O	2.19	0.41
1:A:322:GLU:HG3	1:A:322:GLU:H	1.47	0.41
1:A:308:GLU:CD	1:A:311:ARG:HH11	2.24	0.41
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.55	0.41
1:A:131:ASN:ND2	1:A:131:ASN:C	2.72	0.41
1:A:290:GLU:H	1:A:290:GLU:HG3	1.40	0.41
1:A:87:ASN:HB3	6:A:702:BOG:H3	2.03	0.41
1:A:470:PHE:CD2	1:A:525:LEU:HD22	2.56	0.41
1:B:2179:GLU:O	1:B:2185:ARG:NH2	2.54	0.41
1:B:2173:ASP:O	1:B:2177:VAL:HG23	2.21	0.41
1:A:444:VAL:O	1:A:444:VAL:CG1	2.69	0.41
1:B:2206:THR:HG21	1:B:2385:TYR:CE2	2.55	0.41
1:A:386:HIS:CE1	6:A:704:BOG:H1'2	2.56	0.40
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.86	0.40
1:B:2168:ASN:C	1:B:2170:GLU:N	2.74	0.40
1:B:2131:ASN:HD22	1:B:2134:TYR:H	1.69	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:B:2185:ARG:HE	1:B:2438:ARG:HD3	1.86	0.40
1:B:2092:ILE:HA	1:B:2096:PHE:HE1	1.86	0.40
1:A:168:ASN:C	1:A:170:GLU:N	2.74	0.40
1:A:582:VAL:O	1:A:583:GLN:C	2.60	0.40
1:B:2183:LEU:HA	1:B:2183:LEU:HD23	1.84	0.40
1:A:388:HIS:C	1:A:390:LEU:N	2.75	0.40
1:A:344:VAL:O	1:A:349:VAL:HG23	2.22	0.40
1:B:2452:ILE:O	1:B:2456:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	522 (95%)	24 (4%)	4 (1%)	30	43
1	B	550/552 (100%)	516 (94%)	30 (6%)	4 (1%)	30	43
2	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1107/1113 (100%)	1045 (94%)	54 (5%)	8 (1%)	30	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	B	2121	SER
1	B	2122	TYR
1	A	514	PRO
1	B	2514	PRO
1	A	398	GLU
1	B	2435	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/492 (100%)	445 (90%)	47 (10%)	12	17
1	B	492/492 (100%)	442 (90%)	50 (10%)	11	15
2	F	7/7 (100%)	6 (86%)	1 (14%)	5	5
All	All	991/991 (100%)	893 (90%)	98 (10%)	11	16

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	54	GLN
1	A	56	LYS
1	A	93	LEU
1	A	99	VAL
1	A	101	ASN
1	A	117	LEU
1	A	120	ARG
1	A	123	LEU
1	A	131	ASN
1	A	137	LYS
1	A	171	LEU
1	A	178	LEU
1	A	203	GLN
1	A	230	LEU
1	A	238	LEU
1	A	239	ASP
1	A	252	LEU
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL
1	A	294	LEU
1	A	295	VAL
1	A	298	LEU
1	A	300	MET
1	A	310	GLN
1	A	311	ARG
1	A	322	GLU
1	A	352	LEU
1	A	369	GLN
1	A	377	ILE
1	A	385	TYR
1	A	406	GLN
1	A	408	LEU
1	A	412	SER
1	A	416	GLU
1	A	419	LEU
1	A	422	PHE
1	A	444	VAL
1	A	459	LYS
1	A	484	GLU
1	A	509	VAL
1	A	525	LEU

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Mol	Chain	Res	Type
1	A	534	LEU
1	A	543	GLN
1	A	579	SER
1	A	583	GLN
1	B	2034	ASN
1	B	2054	GLN
1	B	2056	LYS
1	B	2093	LEU
1	B	2099	VAL
1	B	2101	ASN
1	B	2117	LEU
1	B	2120	ARG
1	B	2123	LEU
1	B	2131	ASN
1	B	2137	LYS
1	B	2171	LEU
1	B	2178	LEU
1	B	2180	LYS
1	B	2230	LEU
1	B	2238	LEU
1	B	2239	ASP
1	B	2248	LYS
1	B	2252	LEU
1	B	2272	GLU
1	B	2289	GLN
1	B	2290	GLU
1	B	2291	VAL
1	B	2294	LEU
1	B	2298	LEU
1	B	2300	MET
1	B	2310	GLN
1	B	2311	ARG
1	B	2322	GLU
1	B	2352	LEU
1	B	2369	GLN
1	B	2377	ILE
1	B	2385	TYR
1	B	2397	ILE
1	B	2398	GLU
1	B	2406	GLN
1	B	2409	TYR
1	B	2412	SER

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Mol	Chain	Res	Type
1	B	2416	GLU
1	B	2419	LEU
1	B	2422	PHE
1	B	2444	VAL
1	B	2459	LYS
1	B	2484	GLU
1	B	2509	VAL
1	B	2525	LEU
1	B	2534	LEU
1	B	2543	GLN
1	B	2579	SER
1	B	2583	GLN
2	F	2596	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	131	ASN
1	A	386	HIS
1	A	417	HIS
1	A	429	GLN
1	A	454	GLN
1	A	464	ASN
1	B	2034	ASN
1	B	2131	ASN
1	B	2242	HIS
1	B	2386	HIS
1	B	2400	GLN
1	B	2417	HIS
1	B	2429	GLN
1	B	2454	GLN
1	B	2464	ASN
2	F	2601	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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
3	NAG	A	661	1,3	12,14,15	0.69	0	15,19,21	0.80	1 (6%)
3	NAG	A	662	3	12,14,15	0.79	0	15,19,21	0.74	0
4	NAG	A	671	1,4	12,14,15	0.54	0	15,19,21	0.78	0
4	NAG	A	672	4	12,14,15	1.77	1 (8%)	15,19,21	3.06	4 (26%)
4	MAN	A	673	4	10,11,12	1.00	1 (10%)	11,15,17	1.22	2 (18%)
4	MAN	A	674	4	10,11,12	1.88	3 (30%)	11,15,17	1.20	3 (27%)
3	NAG	B	2661	1,3	12,14,15	0.79	0	15,19,21	0.90	1 (6%)
3	NAG	B	2662	3	12,14,15	0.74	0	15,19,21	0.76	0
4	NAG	B	2671	1,4	12,14,15	0.63	0	15,19,21	0.93	0
4	NAG	B	2672	4	12,14,15	1.13	1 (8%)	15,19,21	2.70	3 (20%)
4	MAN	B	2673	4	10,11,12	0.92	1 (10%)	11,15,17	1.15	1 (9%)
4	MAN	B	2674	4	10,11,12	1.94	3 (30%)	11,15,17	1.22	1 (9%)

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	661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	662	3	-	0/6/23/26	0/1/1/1
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	MAN	A	673	4	-	0/2/19/22	0/1/1/1
4	MAN	A	674	4	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2662	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2672	4	-	0/6/23/26	0/1/1/1
4	MAN	B	2673	4	-	0/2/19/22	0/1/1/1
4	MAN	B	2674	4	1/1/4/5	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	672	NAG	C8-C7	5.70	1.62	1.50
4	B	2674	MAN	C4-C5	3.78	1.61	1.53
4	A	674	MAN	C4-C5	3.78	1.61	1.53
4	B	2672	NAG	C8-C7	3.33	1.57	1.50
4	B	2674	MAN	O5-C5	3.04	1.51	1.45
4	A	674	MAN	C3-C2	2.93	1.59	1.52
4	B	2674	MAN	C3-C2	2.81	1.59	1.52
4	A	674	MAN	O5-C5	2.64	1.50	1.45
4	A	673	MAN	C6-C5	2.43	1.60	1.52
4	B	2673	MAN	C6-C5	2.19	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	672	NAG	C8-C7-N2	-9.22	98.08	116.11
4	B	2672	NAG	C8-C7-N2	-7.78	100.90	116.11
4	A	672	NAG	C3-C2-N2	-5.14	103.93	111.76
4	B	2672	NAG	O7-C7-C8	-4.62	113.02	122.04
4	A	672	NAG	O7-C7-C8	-4.52	113.23	122.04
4	B	2672	NAG	C3-C2-N2	-4.45	104.99	111.76
4	A	673	MAN	O6-C6-C5	2.88	121.28	111.36
4	B	2673	MAN	O6-C6-C5	2.84	121.14	111.36
4	B	2674	MAN	O5-C5-C6	2.40	109.50	106.98
3	B	2661	NAG	C3-C2-N2	-2.29	108.27	111.76
4	A	672	NAG	C2-N2-C7	-2.21	119.38	123.09
4	A	674	MAN	O5-C5-C6	2.08	109.16	106.98
4	A	674	MAN	C4-C3-C2	2.08	113.29	110.50
3	A	661	NAG	C3-C2-N2	-2.07	108.61	111.76
4	A	674	MAN	O5-C5-C4	2.03	113.23	110.65
4	A	673	MAN	O5-C5-C4	2.02	113.22	110.65

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2674	MAN	C1
4	A	674	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

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$
5	NAG	A	681	1	12,14,15	0.55	0	15,19,21	1.09	1 (6%)
7	ACD	A	701	-	21,21,21	0.83	0	21,21,21	0.77	0
6	BOG	A	702	-	20,20,20	0.82	1 (5%)	25,25,25	0.70	0
6	BOG	A	703	-	20,20,20	0.88	0	25,25,25	0.70	0
6	BOG	A	704	-	20,20,20	0.90	2 (10%)	25,25,25	0.67	0
5	NAG	B	2681	1	12,14,15	0.77	0	15,19,21	1.04	1 (6%)
7	ACD	B	2701	-	21,21,21	0.69	0	21,21,21	0.66	0
6	BOG	B	2702	-	20,20,20	0.66	0	25,25,25	0.63	0
6	BOG	B	2704	-	20,20,20	0.82	2 (10%)	25,25,25	0.66	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
5	NAG	A	681	1	-	0/6/23/26	0/1/1/1
7	ACD	A	701	-	-	0/19/19/19	0/0/0/0
6	BOG	A	702	-	-	0/11/31/31	0/1/1/1
6	BOG	A	703	-	-	0/11/31/31	0/1/1/1
6	BOG	A	704	-	-	0/11/31/31	0/1/1/1
5	NAG	B	2681	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ACD	B	2701	-	-	0/19/19/19	0/0/0/0
6	BOG	B	2702	-	-	0/11/31/31	0/1/1/1
6	BOG	B	2704	-	-	0/11/31/31	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	BOG	O5-C1	2.34	1.47	1.41
6	A	704	BOG	O1-C1	2.25	1.44	1.40
6	B	2704	BOG	O5-C1	2.21	1.47	1.41
6	B	2704	BOG	O1-C1	2.07	1.43	1.40
6	A	702	BOG	O5-C1	2.03	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	681	NAG	C3-C2-N2	-2.54	107.89	111.76
5	B	2681	NAG	C8-C7-N2	-2.32	111.56	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/552 (100%)	-0.40	9 (1%) 68 67	14, 26, 43, 56	0
1	B	552/552 (100%)	-0.34	10 (1%) 65 63	12, 27, 46, 61	0
2	F	9/9 (100%)	2.02	5 (55%) 0 0	52, 55, 66, 71	0
All	All	1113/1113 (100%)	-0.35	24 (2%) 54 57	12, 27, 46, 71	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2409	TYR	7.2
2	F	2603	SER	7.0
1	A	74	PHE	4.2
1	B	2583	GLN	3.9
1	B	2074	PHE	3.7
1	A	399	ASP	3.4
1	A	75	LEU	2.7
2	F	2599	THR	2.7
2	F	2601	ASN	2.5
1	B	2274	ILE	2.5
1	B	2294	LEU	2.5
1	B	2075	LEU	2.3
1	B	2214	HIS	2.3
1	A	80	LEU	2.3
2	F	2600	ILE	2.3
1	A	52	PHE	2.2
1	A	583	GLN	2.2
1	A	122	TYR	2.2
1	A	107	PHE	2.2
1	A	409	TYR	2.1
1	B	2081	LEU	2.1
1	B	2215	LYS	2.0
1	B	2399	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	2595	THR	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	672	14/15	0.31	-	46,52,55,57	0
4	NAG	B	2671	14/15	0.15	-	27,29,34,41	0
3	NAG	A	662	14/15	0.52	-	64,67,70,72	0
4	MAN	B	2674	11/12	0.73	-	78,80,82,82	0
3	NAG	A	661	14/15	0.20	-	44,50,53,58	0
3	NAG	B	2662	14/15	0.71	-	68,71,74,75	0
4	NAG	B	2672	14/15	0.31	-	49,55,57,62	0
4	MAN	A	673	11/12	0.34	-	60,62,65,67	0
3	NAG	B	2661	14/15	0.34	-	52,54,58,64	0
4	MAN	A	674	11/12	0.37	-	70,71,72,72	0
4	NAG	A	671	14/15	0.12	-	28,30,33,39	0
4	MAN	B	2673	11/12	0.38	-	66,67,72,76	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	BOG	B	2702	20/20	0.29	-	40,45,47,47	0
5	NAG	A	681	14/15	0.41	-	58,61,64,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACD	B	2701	22/22	0.15	-	19,25,29,32	0
7	ACD	A	701	22/22	0.15	-	18,22,28,31	0
5	NAG	B	2681	14/15	0.47	-	68,70,71,72	0
6	BOG	A	702	20/20	0.30	-	38,50,54,54	0
6	BOG	B	2704	20/20	0.23	-	32,61,64,65	0
6	BOG	A	703	20/20	0.14	-	33,44,46,47	0
6	BOG	A	704	20/20	0.33	-	42,63,65,67	0

## 6.5 Other polymers

There are no such residues in this entry.